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Scattering of Electrons by Hydrogenic Ions.

Najib Nimer Abusalbi
Louisiana State University and Agricultural & Mechanical College

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SCATTERING OF ELECTRONS BY HYDROGENIC IONS

The Louisiana State University and Agricultural and Mechanical Col. PH.D. 1981

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SCATTERING OF ELECTRONS BY HYDROGENIC IONS

A Dissertation

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in

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Najib Nimer AbuSalbi
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M.S., Louisiana State University, 1978
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To My Wife and Daughter

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ABSTRACT

The "Algebraic Variational" method in Atomic physics is applied for the first time to the scattering (both elastic and inelastic) of electrons by highly stripped (hydrogenic) atomic ions. The overall behavior of the excitation 1s→2s and 1s→2p cross sections is investigated using a 6 state expansion (1s-2s-2p) one and two p pseudostates) of the target wave function. The close coupling calculation is carried out up to a total angular momentum L_{MAX}, ($L_{MAX} \leq 5$) and for energies ranging from just above the n=2 threshold to 5 times threshold; otherwise the Coulomb Born approximation with exchange is used. The computed collision strengths are then fit by an analytic formula. Finally, using a large pseudostate set, resonances between the n=2 and n=3 thresholds are investigated and accurately traced. Resonance enhancement of excitation rates is discussed. Results are reported for electron scattering by C^{5+} and O^{7+}. Comparison is made to other theoretical calculations.

CHAPTER I

INTRODUCTION

The study of atomic processes in high temperature plasmas, both laboratory and interstellar, has grown into an increasingly important subject. Experimental and theoretical research is being conducted in order to interpret and comprehend the nature of these processes which occur in a hot fused plasma in a tokamak or in an interstellar medium. The investigation of spectral lines from these and other similar systems, reveals the presence of highly stripped heavy ions. For instance, in a hot confined plasma, elements like C, O and Fe are continuously excited by electron impact, thus forming all sorts of ions up to the hydrogen like. There exists now an increasing necessity for a full comprehension of the complicated structures resulting from the electron impact excitation of ions.

This work presents a physical framework for the electron impact excitation of hydrogenic ions in the energy range from just above, to around twenty times the first excitation threshold. The theory is basically a close coupling calculation which employs the "Algebraic Variational" method.[1,2,3] Recent reviews of the method discuss the principles and the applications (so far made) of the different Kohn-type variational techniques. Most

existing applications are to the excitation of the neutral atoms of H and He; a few have been made to alkali metals and the atoms of C, N and O, and one application to elastic scattering from He^+.[4] Emphasis has been placed recently on He^+,[5-8] where a large discrepancy in the 1s→2s excitation cross section, exists between theory and experiment. Besides, a 3 state close coupling calculation has been made on the highly stripped ion Fe^{25+}.[9] A major objective of the work is to answer the questions: (1) what is the importance of pseudostates in close coupling calculations made on ions? (2) which of the common approximation techniques is adequate in solving scattering problems? (3) what is the effect of resonances on excitation rates in hydrogenic ions?

A survey of variational close coupling calculation is presented in Chapter Two. The importance of pseudostates is also discussed, as well as the problem associated with their choice. The degree of agreement between the different variational formulas of the K matrix (The "Kohn" (K), the "Inverse-Kohn" (IK), the "Optimized Anomaly Free" (OAF), the "Optimized Minimum Norm" (OMN) and its "Inverse" (IOMN)) is also discussed. The problems of anomalies in variational methods and pseudoresonances near pseudostate thresholds are considered.

In Chapter Three, the basic matrix elements with all associated integrals are evaluated. The evaluation of these quantities has been discussed previously for neutral systems.[10,11,12] This text considers the problem for one electron ions.

Results for the hydrogenic ions C^{5+} and O^{7+} are presented in Chapter Four. These ions are intrinsically important in high temperature plasmas. They may also be used as the low Z-limit for isoelectronic scaling to higher Z elements. The excitation 1s→2s and 1s→2p, as well as the elastic cross sections are calculated and compared with results of other theoretical calculations. These latter include standard close coupling calculations (3cc),[6,13,14,15] distorted wave with exchange (DW),[15,16] infinite Z hydrogenic (IZH)[18] approximation, as well as the simple Coulomb Born (CB)[19] and Coulomb Born with exchange (CBX) approximations.[18] We were not aware of any experimental results on these ions at the time this work was in progress. Finally, resonances between the n=2 and n=3 hydrogenic levels are investigated. The calculated positions and widths compare well with those obtained by the complex rotation method. Previous calculations quoted in a review by Henry,[20] have demonstrated the special importance of resonance contribution to rate coefficients of optically forbidden excitations, the 1s→2s excitation for example. We determine in this work that resonance

of excitation rates is not as important as previously estimated by Seaton.[14,21]

General conclusions are stated in Chapter Five. A complete set of computer programs is included in Appendix G. Some subprograms which are taken from existing programs for electron hydrogen scattering (using the same approach) by Callaway et al., are also included.

CHAPTER II

SURVEY OF THEORY

In this chapter we review the basic formalism involved in the application of the variational method to the problem of electron scattering by an atomic ion, on the basis of a close couling expansion with pseudostates.

A. General Principles

We consider an external electron incident on an N-electron target of nuclear charge Z, and denote by "z" the net charge

$$z = Z - N \tag{2.1}$$

We will restrict the discussion to non-relativistic situations in which the total angular momentum L, the total spin S, and the total parity π are separately conserved. In the present work, the ion is always initially in its ground state; therefore $\pi = (-1)^L$.

The total wave function of the N+1 electron system is denoted by Ψ_a where "a" specifies an independent particular solution of the Schrodinger equation

$$H\Psi_a = E\Psi_a \tag{2.2}$$

in which H is the total Hamiltonian of the system and E is its total energy. The wave function satisfies scattering boundary conditions. An incoming wave in channel "a" results in outgoing waves in all accessible channels. A particular channel "j" is characterized by the set of quantum numbers describing the target states (the principal quantum number n_j, the orbital angular momentum L_j, its azumithal component m_{L_j}, the spin S_j, etc. and the orbital angular momentum ℓ_j and wave vector k_j of the projectile:

$$k_j^2 = E - E_j \tag{2.3}$$

where E_j is the energy of the target state j. The spins and angular momenta satisfy the triangular inequalities

$$|L_j-\ell_j| \leq L \leq L_j+\ell_j \tag{2.4}$$

and

$$|S_j - 1/2| \leq S \leq S_j + 1/2 \quad .$$

The channel, denoted by Γ_j, is said to be closed if $k_j^2 \leq 0$, and open (or accessible) if $k_j^2 > 0$.

B. Pseudostates

We consider here only the case of a two electron system. The total wave function Ψ_a is expanded in a set

of one electron target functions, in which the expansion coefficients are functions of the scattered electron coordinates. Let $\vec{x}$ denote the coordinates and spin of an electron, then

$$\Psi_a(\vec{x}_1,\vec{x}_2) = A\sum_j \psi_j(\vec{x}_1)F_{ja}(\vec{x}_2) \tag{2.5}$$

where A is the antisymmetry operator.

A close coupling expansion is used. This restricts the functions ψ_j to a finite set of exact target eigenstates as well as pseudostates. The choice of pseudostates is made by requiring that the target Hamiltonian (H_T) be diagonalized in the subspace spanned by the selected set of orthogonal functions, that is

$$\int \psi_j^*,(\vec{x}_1)\ [H_T - E_j\delta_{jj},]\psi_j(\vec{x}_1)d\tau_1 = 0 \tag{2.6}$$

The functions ψ_j are constructed as a linear combination of specified basis functions, and are only eigenfunctions of H_T within the subspace spanned by the basis elements. Consider, for instance, a target state of specific angular momentum L_j, then the radial Hamiltonian is given by

$$H_{L_j}(r) = -\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{L_j(L_j+1)}{r^2} - 2\frac{Z}{r}\ .$$

Consider also a set of n Slater type functions

$$\eta_i(r) = r^{m_i} e^{-\zeta_i r}$$

The functions

$$R_j(r) = \sum_{i=1}^{n} C_{j,i}\, \eta_i(r) \qquad (2.7)$$

form a set of orthogonal functions that can be normalized by imposing some condition on the coefficients $C_{j,i}$; they are the eigenfunctions of H_{L_j} within the subspace of η_i's.

The diagonalization procedure yields a set of energies (E_j), powers (m_j) of r, exponents (ζ_j), and coefficients ($C_{j,i}$) which define the radial target functions $R_j(r)$ (the radial part of ψ_j). For example, for $L_j = 0$, if the basis includes the functions e^{-Zr}, $e^{-Zr/2}$ and $re^{-Zr/2}$, Eq. (2.6) yields the exact hydrogenic 1s and 2s states and a third state ($\overline{3s}$) which is a combination of η_i's. Functions of the type ψ_j, which are not exact target eigenstates are referred to as pseudostates. The term "pseudobasis" is given to the set of the short-ranged functions in which the pseudostates are expanded.

Pseudostates simulate, in an approximate manner, the effect of high bound and continuum states which exist in the real system. Previous calculations on electron

scattering by atoms have shown that pseudostates, when properly chosen, can fully describe the target polarization.[22,23,24] In addition, pseudochannels, once open, absorb some amount of the outgoing flux, resulting in a reduction in the excitation cross sections, in comparison with a close coupling calculation in which only the physical target states are included.[1,4,6,7,25,26] Finally, cross sections (σ_{ps}) for excitations of pseudostates contain information concerning ionization (the excitation of continuum states). An approximate expression for the ionization cross section (σ_I) for a set of pseudostates $|ps\rangle$ and bound states $|b\rangle$ at some energy E, is given by[27,28]

$$\sigma_I(E) = \sum_{\text{pseudostates}} \left[1 - \sum_{\substack{\text{bound}\\ \text{states}}} |\langle b|ps\rangle|^2\right] \sigma_{ps}(E) \quad . \tag{2.8}$$

Thix expression is valid at energies located away from thresholds.

For our purposes, two different sets of pseudostates are used. The first is a six state set consisting of 3s-type functions and 3p-type functions. These are the exact hydrogenic 1s, 2s and 2p states plus 3 pseudostates (one $\bar{s}$-type and two $\bar{p}$-type). It is employed in the energy range from just above the n=3 threshold to

about five times the first excitation threshold. It was necessary to restrict the close coupling expansion to such a small set for two important reasons. One is the amount of computer time it takes to do a single calculation when all pseudochannels are open at relatively high energies; the other is the complicated pseudoresonance problem associated with pseudostate[28,29] expansions as shall be discussed later in the text. Besides, this basis has been shown in a previous work, to yield rather satisfactory results for electron impact excitation of He^+,[7] in comparison to other bases used in different close coupling techniques, in the intermediate energy range where a serious conflict occurs with experiment. Energies and parameters of this basis are listed in Table I. However this small basis is not adequate to describe resonances between the n=2 and n=3 hydrogenic levels. Based on the work of Morgan et al.,[6] a larger basis (14 states) which contains the exact 1s, 2s, 3s, 2p, 3p and 3d states and 8 pseudostates (three $\bar{s}$-type, three $\bar{p}$-type, one $\bar{d}$-type and one $\bar{f}$-type), is used in that energy region. Energies and parameters of this basis are also given in Table I.

We draw the attention here to Table I in which we have scaled the pseudobasis exponents by the nuclear charge, and thus the energies scale by Z^2. We also note that the energies listed are those of the pseudostates as defined in Eq. (2.7).

C. Calculation of Total Cross Sections

This and the next section describe the basic features of the variational method employed.[1,2,3]

The total wave function can be written as

$$\Psi_a(\vec{x}_1,\vec{x}_2) = \sum_j G_{ja}(r_2)\,\Phi_j(\vec{x}_1;\hat{r}_2,\sigma_2) \qquad (2.9)$$

in which Φ_j combines the target wave function $\psi_j(\vec{x}_1)$ with the angular and spin functions of the projectile. The function $G_{ja}(r_2)$ is the radial part of the scattering function $F_{ja}(\vec{x}_2)$ which appeared in Eq. (2.5). We will denote the set $(\vec{x}_1;\hat{r}_2;\sigma_2)$ by γ_j. The antisymmetrization operator can be expressed in terms of the permutation operator P_{12}

$$= (1 \pm P_{12})/\sqrt{2} \quad . \qquad (2.10)$$

The signs here stand for triplet (-) states in which the electron spins are aligned, and singlet (+) states in which these spins are antiparallel.

In each channel Γ_j, the variational function $G_{ja}(r)$ obeys the proper boundary conditions for small r

$$G_{ja}(r) \underset{r\to 0}{\to} r^{\ell_j} \quad , \qquad (2.11)$$

as well as for large r

$$G_{ja}(r) \underset{r\to\infty}{\to} k_j^{-1/2}\, e^{-|k_j|r}/r\ , \quad \text{if } k_j^2 \le 0$$

$$G_{ja}(r) \underset{r\to\infty}{\to} k_j^{-1/2}(\delta_{ja} \sin \zeta_i + K_{ja} \cos \zeta_i)/r$$

$$\text{if } k_j^2 > 0 \qquad (2.12)$$

in which

$$\zeta_j = k_j r - \ell_j\, \pi/2 + (z/k_j) \ln 2k_j r + \sigma_j\ . \qquad (2.13a)$$

Here σ_j is the Coulomb phase defined by

$$\sigma_j = \text{Arg}\ \Gamma(\ell_j + 1 - iz/k_j)\ . \qquad (2.13b)$$

The quantities K_{ja} in Eq. (2.12) are elements of the reactance (or K) matrix.

In order to satisfy these conditions, we expand the scattering function in the following manner

$$G_{ia}(r) = \sum_{s=1}^{2} (\alpha_s)_{ia}\, f_s(k_i,r) + \sum_{\nu=1}^{n_c} C_{ia,\nu}\, \eta_\nu^{(i)}(r)$$

(2.14)

in which f_s is a long range energy dependent function; $C_{ia,\nu}$ is an expansion coefficient; $\eta_\nu(r)$ is a short range square integrable function (usually a Slater orbital) which decays at least as fast as $1/r^2$ for large r; n_c is the number of elements in the short range basis; and α_s (s = 1,2) are matrices whose choice depends on the particular variational method used; for instance, the Kohn choice is

$$(\alpha_1)_{ia} = \delta_{ia} \qquad (\alpha_2)_{ia} = K_{ia} \ , \tag{2.15a}$$

while the Inverse-Kohn choice is

$$(\alpha_1^{-1})_{ia} = K_{ia} \qquad (\alpha_2)_{ia} = \delta_{ia} \ . \tag{2.15b}$$

Unlike the situation involving an atomic target, the net charge of the system is not zero. The long range functions, f_1 and f_2, can no longer be Bessel functions, but must approach Coulomb functions asymptotically. We have chosen f_1 and f_2 as

$$\begin{aligned} f_1(k_i,r) &\; k_i^{-1/2} \; F_{\ell_i}(k_i,r)/r \\ f_2(k_i,r) &= k_i^{-1/2}(1-e^{-\gamma r})^{2\ell_i+1} \; G_{\ell_i}(k_i,r)/r \end{aligned} \tag{2.16}$$

in which F_ℓ and G_ℓ are, respectively, the regular and

irregular solutions of the Coulomb differential equation

$$\left[\frac{d^2}{dr^2} - \frac{2\alpha k}{r} - \frac{\ell(\ell+1)}{r^2} + k^2 \right] U(\ell,kr) = 0 \qquad (2.17)$$

where α is the Coulomb parameter defined by

$$\alpha = - \frac{z}{k} = \frac{-(Z-1)}{k} \quad . \qquad (2.18)$$

For small r, F_ℓ and G_ℓ behave as $r^{\ell+1}$ and $r^{-\ell}$ respectively. The multiplicative factor introduced in Eq. (2.16) regularizes f_2 such that both f_1 and f_2 go to zero as r^ℓ when r approaches the origin. In the asymptotic region, F_ℓ and G_ℓ behave as

$$F_\ell \underset{r\to\infty}{\sim} \sin \xi(r)$$

$$G_\ell \underset{r\to\infty}{\sim} \cos \xi(r) \qquad (2.19)$$

which complies with the conditions imposed by Eq. (2.12).

The outcome of the scattering problem must be stable with respect to the choice of the parameter, γ. Thus an optimization procedure is carried out for each target. In fact, calculated cross sections, eigenphases, as well as other physical quantities, should be stable over a considerable range of values of γ. An optimum γ has been found for each target. Examples of the optimization

procedure are illustrated in Appendix A.

The partial cross section for a definite L, S and π, is proportional to the square of the transition (or T) matrix which is related to the K matrix by

$$T = \frac{2iK}{1-iK} \quad . \tag{2.20}$$

The partial excitation cross section from state i to state j is then given by

$$\sigma_{LS\pi}(i \to j) = \frac{1}{2k_i^2} (2L+1)(2S+1) \sum_{\ell_i \ell_j} \frac{1}{(2L_i+1)(2S_i+1)} |T_{ij}(L,S,\pi)|^2 \quad , \tag{2.21}$$

and the total cross section is obtained by summing over L, S and π

$$\sigma(i \to j) = \sum_{L,S,\pi} \sigma_{LS\pi}(i \to j) \tag{2.22}$$

Cross sections are expressed in units of πa_o^2 (a_o is the Bohr radius).

D. Variational Methods

The basic procedure employed in solving the set of coupled integro-differential equations,[1] consists of

writing an expansion for the trial scattering function $G_{ia}(r)$, as given in Eq. (2.14). The reactance matrix elements (K_{ij}) are then expressed in terms of the matrix elements "M^{ij}_{st}" which constitute the central part of the algebraic variational method (i and j specify the channel indices and s and t specify the long range functions). These matrix elements can be expressed as

$$M^{ij}_{st} = F^{ij} - \sum_{m\mu n\nu} M^{im}_{s\mu} (B^{-1})^{mn}_{\mu\nu} M^{nj}_{\nu t} \quad , \qquad (2.23)$$

$(m, n = 1,2,\ldots,n_o \; ; \quad \mu,\nu = 1,2,\ldots,n_c)$.

Here n_o is the number of open channels in the final state. The terms appearing in this equation are defined below.

(i) the bound-bound matrix elements

$$B^{mn}_{\mu\nu} = (\eta_\mu(r)\,\Phi(\gamma_m) \,|(H-E)(1\pm P_{12})\,|\Phi(\gamma_n)\,\eta_\nu(r)) \quad , \qquad (2.24)$$

(ii) the bound-free matrix elements

$$M^{im}_{\mu s} = (\eta_\mu(r)\,\Phi(\gamma_m) \,|(H-E)(1\pm P_{12})\,|\Phi(\gamma_i) f_s(k_i,r)) \quad ,$$

(2.25)

and (iii) the free-free matrix elements

$$F_{st}^{ij} = (f_s(k_i,r)\Phi(\gamma_i)|(H-E)(1\pm P_{12})|\Phi(\gamma_j)f_t(k_j,r)) \ . \tag{2.26}$$

The evaluation of these matrix elements will be discussed in detail in the next chapter.

The Kohn variational method expresses the K matrix element as

$$K_{ab} = -M_{11}^{ab} - \sum_{jk} M_{21}^{ka} \ (M_{22}^{-1})^{k}_{j} \ M_{21}^{jb} \tag{2.27}$$

$(a,b,j,k = 1,2,\ldots,n_o)$,

in which the error is only of the second order in the error of the function $G_{ia}(r)$. Similarly the Inverse-Kohn expression is

$$(K^{-1})_{ab} = M_{22}^{ab} - \sum_{jk} M_{12}^{ka} \ (M_{11}^{-1})^{k}_{j} \ M_{12}^{jb} \ . \tag{2.28}$$

It is obvious that both expressions, (2.27) and (2.28), suffer from severe anomalies whenever the inverted matrices are singular or nearly so. Such anomalies which occur at some particular energies may be avoided by adjusting the basis functions, or using Nesbet's

criterion, according to which the Kohn formula is preferred to the Inverse-Kohn if the ratio $|\text{Det } M_{22}/\text{Det } M_{11}|<1$, and vice versa (Det stands here for the "determinant of").

Besides, the OMN method[30,31] and its inverse IOMN still apply the Kohn and Inverse Kohn formulas, but to a transformed matrix M'. Anomalies still occur at energies where the matrices M'_{22} and M'_{11} have vanishing determinants. Finally, the OAF method, introduced by Nesbet[32] has been constructed in a manner that avoids the anomalies associated with the other methods. The basic procedure is to reduce M to its upper triangular form by a unitary transformation,[33] with the assumption that all the eigenvalues of M are real. It turns out that the OAF procedure possesses anomalies of its own, frequently manifest when the K matrix becomes significantly assymetric (the OAF K matrix need not be symmetric in some energy regions except in the limits of an exact solution).

The degree of agreement, or disagreement between the different methods clearly depends on the presence of anomalies which arise in some partial waves at some energies. Table II shows examples in which agreement varies from excellent to fair, even to poor. For instance, the IOMN value has a bad anomaly for L = 0, S = 1. This value is excluded from the averaging procedure

done in order to obtain a best estimate of the cross section. The same holds true for the OAF value for L = 5, S = 1. This degree of agreement between the variational methods seems to be consistent with our aim to achieve a 1% accuracy in the calculated cross sections. The example shown in Table II shows an uncertainty of 0.4% in the total cross section ($L \leq 5$).

E. Pseudoresonances. The K Matrix Fit

A major difficulty associated with the use of pseudobases, arises near artificial pseudothresholds where broad pseudoresonances occur.[29] In previous work, this problem has been avoided by altering the parameters of the basis set so as to shift the position of the resonance away from the energy region of interest. Recently, Burke et al.[34] suggested an alternative approach in which the transition amplitude is effectively averaged over the resonance region by means of a fit to a low order polynomial in k_i^2 (the incident energy)

$$f_{ij} = a\, k_i^4 + b\, k_i^2 + c \qquad (2.29)$$

where a, b and c are complex.

We applied this approach and made linear least squares fits to average over the severe pseudoresonance associated with the 3s-3p basis, which occurs at

approximately $k_i^2 = 38.6$ Ry below the pseudothreshold at 47.2 Ry in the ^1S partial wave in C^{5+}. It turned out that the reliability of the method depends to a certain extent on the number of points at which the fit is made. This is an undesirable aspect when expensive close coupling calculations are involved. Consequently, we decided to use the procedure related to that used by Callaway et al. in previous work on electron impact excitation of C^{3+}.[35]

This procedure is based on the work of Eissner and Seaton.[36] The essential point is that the real K matrix acquires a pole at some energy E_λ in the vicinity of the resonance (or pseudoresonance) where for fixed L and S, it can be expressed as

$$K_{ij}(E) = K_{ij}^{(0)}(E) + C_{ij}/(E_\lambda - E) \quad . \tag{2.30}$$

The first term on the right represents the background and the second represents the pole contribution. It has been established in the formal resonance theory, that residues of the transition matrix and consequently of the K matrix can be factored near a pole (this is due to the behavior of the scattering Green's function near that pole); we then have

$$C_{ij} = C_i \, C_j \quad . \tag{2.31}$$

Hence, in the presence of one or more poles, we fit our calculated K matrices to the analytic equation in x (the scaled energy defined as the ratio of the incident energy to the n=2 excitation threshold)

$$K_{ij}(x) = \sum_{n=0}^{N} D_{ij}^{(n)} (x-x_o)^n + \sum_{\lambda} \frac{C_{ij}^{(\lambda)}}{x_\lambda - x} \quad . \tag{2.32}$$

Here x_o is conveniently chosen to be the lowest energy in the region under investigation, and N is the number of terms considered in the background representation. N is varied until an acceptable fit is obtained. For most cases, a linear (N=1) or at most quadratic (N=2) representation of the background is sufficient.

In fact, the fitting procedure is not as complicated as Eq. (2.32) may suggest. Once the poles are accurately located from simple ab initio calculations, only a linear least squares fit would then be required to determine the coefficients $D_{ij}^{(n)}$ and the residues $C_{ij}^{(\ )}$. We found it helpful to test the quality of the fits by checking the validity of the factorization property of the residues given by Eq. (2.31).

In order to compare this method with that of Burke et al., we considered the same case mentioned above. The contribution of the existing pole (at x = 1.431) is dropped after the fitting is completed, and the transition amplitudes, as well as the cross sections,

are recalculated using only the background representation of the K matrix. Figs. I and II show the behavior of the real and imaginary parts of the transition amplitude for the 2s excitation. The dark dots (connected by a light line) are the calculated values which show a rapid variation of this amplitude that results in a rapid variation in the cross section, shown in Fig. III. The dashed lines show the results produced by Burke's method, while the solid lines show the results produced by the procedure described above (K matrix fit). The same procedures have also been applied to the 2p excitation cross section (shown in Fig. IV),[37] as well as for the 2s and 2p ^1S excitation cross sections of O^{7+} in which a pseudoresonance occurs around x = 1.41 in the same energy region. These pseudoresonances seemed to be the only ones of significant effect on the calculated cross sections above ionization.

In conclusion, both methods agree rather well, particularly when it comes to fitting the imaginary part of the transition amplitude. In regard to the real part, the least squares fit tends to fall too low at energies below the resonance and is high at energies above the resonance. This results in cross sections that are too large or too small in the energy regions indicated above. We think that the least squares fit would be improved by having more calculated

points evenly spaced about the pole. That method appears to be less suitable when only a relatively small amount of data is available, as in the present calculations. A fit to the K matrix apparently requires less data to yield satisfactory results.

CHAPTER III

EVALUATION OF MATRIX ELEMENTS

In this chapter we discuss the evaluation of matrix elements which arise from the application of the algebraic variational method to the scattering of an electron by a one-electron atomic ion of nuclear charge Z. The evaluation of these matrix elements has already been discussed in the case of neutral targets.[10,11,12] Section A introduces the principal types of matrix elements, while Section B evaluates the specific integrals involved in the variational matrices.

A. Principal Types of Matrix Elements

We define the total wave function of the two-electron system, of definite L and M (the z-component of L)

$$\Psi_a(\vec{x}_1,\vec{x}_2) = 2^{-\frac{1}{2}}(1 \pm P_{12}) \sum_i (\ell_i\ I_i\ m_i\ M_i|LM)\ \Psi_i(\vec{r}_1)\ F_{ia}(\vec{r}_2) \tag{3.1}$$

in which $(\ell_i\ L_i\ m_i\ M_i\ LM)$ is a vector coupling coefficient;[38] then we write Ψ_i and F_{ia} in spherical coordinates

$$\begin{cases} \Psi_i(\vec{r}_1) = R_i(\vec{r}_i)\ Y_{L_i}^{M_i}(\Omega_1) \\ F_{ia}(r_2) = G_{ia}(\vec{r}_2)\ Y_{\ell_i}^{m_i}(\Omega_2) \end{cases} \tag{3.2}$$

where $Y_\ell^m(\Omega)$ is a "spherical Harmonic". Eq. (3.1) can now be rewritten as

$$\Psi_a(\vec{x}_1,\vec{x}_2) = 2^{-\frac{1}{2}}(1 \pm P_{12}) \sum_i R_i(r_1)\, G_{ia}(r_2)\, y^M_{L,L_i\ell_i}(\Omega_1\Omega_2) \tag{3.3}$$

in which the 2-body spherical harmonic $y^M_{L,L_i\ell_i}$ combines the angular factors of the 2 electrons

$$y^M_{L,L_i\ell_i}(\Omega_1\Omega_2) = \sum_{m_iM_i} (\ell_i L_i m_i M_i | LM)\, Y^{m_i}_{\ell_i}(\Omega_2)\, Y^{M_i}_{L_i}(\Omega_1). \tag{3.4}$$

It also has the following property

$$y^M_{L,\ell_iL_i}(\Omega_1\Omega_2) = y^M_{L,L_i\ell_i}(\Omega_2\Omega_2) \quad (-1)^{L_i+\ell_i-L} \tag{3.5}$$

The multiplicative factor $\{(-1)^{L_i+\ell_i-L}\}$ is always a unity for the scattering problem in which the parity is $(-1)^L$. Eq. (3.3) can then be rewritten as

$$\begin{aligned}\Psi_a(\vec{x}_1,\vec{x}_2) = 2^{-\frac{1}{2}} \sum_i [&R_i(r_1)\, G_{ia}(r_2)\, y^M_{L,L_i\ell_i}(\Omega_1\Omega_2) \\ &\pm R_i(r_2)\, G_{ia}(r_1)\, y^M_{L,L_i\ell_i}(\Omega_2\Omega_1)]\end{aligned} \tag{3.6}$$

Now we define the variational functional I_{ab}

$$I_{ab} = \int\int \Psi_a(\vec{x}_1,\vec{x}_2)\, [(1 \pm P_{12})(H-E)]\, \Psi_b(\vec{x}_1,\vec{x}_2)\, d\tau_1\, d\tau_2 \tag{3.7}$$

which is related to the M matrix, defined above (see Eq. (2.23)), by

$$I_{ab} = \sum_{s,t=1}^{2} \sum_{k,\ell=1}^{n_o} (\alpha_s)_{ka}\, M^{k\ell}_{st}\, (\alpha_t)_{\ell b} \tag{3.8}$$

in which n_o is the number of open channels, and α_s and α_t are the matrices introduced in Section II.C.

The wave function Ψ_a is not an exact solution of the Schrödinger equation; otherwise, the functional I_{ab} would

identically vanish. Substituting (3.6) in (3.7) we rewrite I_{ab} as

$$I_{ab} = \sum_{i,j=1}^{n_o} \iint \{R_i(r_1)\, G_{ia}(r_2)\, y^M_{L,L_i\ell_i}(\Omega_1\Omega_2) \pm R_i(r_2) \times G_{ia}(r_1)\, y^M_{L,L_i\ell_i}(\Omega_2\Omega_1)\}\, [H\text{-}E]\, R_j(r_1)\, G_{jb}(r_2) \times y_{L,L_j\ell_j}(\Omega_1\Omega_2)\, r_1^2\, r_2^2\, dr_1\, dr_2\, d\Omega_1\, d\Omega_2 \tag{3.9}$$

In order to reduce this expression, it will be convenient to perform the angular integration over the solid angles Ω_1 and Ω_2. For this purpose, we introduce the two operators

$$H_D^{ij}(r_1,r_2) = \iint d\Omega_1\, d\Omega_2\, y^M_{L,L_i\ell_i}(\Omega_1\Omega_2)\, [H\text{-}E]\, y^M_{L,L_j\ell_j}(\Omega_1\Omega_2)$$
$$H_x^{ij}(r_1,r_2) = \iint d\Omega_1\, d\Omega_2\, y^M_{L,L_i\ell_i}(\Omega_2\Omega_1)\, [H\text{-}E]\, y^M_{L,L_j\ell_j}(\Omega_1\Omega_2) \tag{3.10}$$

The total Hamiltonian, H, can be expressed as the sum of 2 single particle Hamiltonians

$$H_i = -\nabla_i^2 - 2\,Z/r_i \qquad (i = 1,2)\ , \tag{3.11a}$$

and an interaction term

$$H_I = 2/r_{12} \tag{3.11b}$$

in which r_{12}^{-1} can be expanded in spherical harmonics

$$r_{12}^{-1} = \sum_{\lambda=0}^{\infty} \frac{r_<^\lambda}{r_>^{\lambda+1}} \frac{4\pi}{2\lambda+1} \sum_{m=-\lambda}^{\lambda} Y_\lambda^{m*}(\Omega_1)\, Y_\lambda^m(\Omega_2) \tag{3.12}$$

where $r_<$ is the smaller and $r_>$ is the larger of $\{r_1,r_2\}$. We would like to note here that atomic units are used

everywhere in this work, and that energies are expressed in Rydbergs unless otherwise specified.

Combining Eqs. (3.11a), (3.11b), and (3.12), and performing the integrations in Eq. (3.10), the radial Hamiltonian operators reduce to

$$H_D^{ij}(r_1,r_2) = \delta_{L_i L_j}\,\delta_{\ell_i \ell_j}\,[T_{\ell_i} + T_{L_i} - 2\frac{Z}{r_1} - 2\frac{Z}{r_2} - E] + \\ + 2\sum_{\lambda} A(\lambda, L_i, \ell_i, L_j, \ell_j)\,\frac{r_<^{\lambda}}{r_>^{\lambda+1}} \qquad (3.13a)$$

$$H_x^{ij}(r_1,r_2) = \delta_{L_i \ell_j}\,\delta_{L_j \ell_i}\,[T_{\ell_i} + T_{L_i} - 2\frac{Z}{r_1} - 2\frac{Z}{r_2} - E] + \\ + 2\sum_{\lambda} A(\lambda, \ell_i, L_i, L_j, \ell_j, L)\,\frac{r_<^{\lambda}}{r_>^{\lambda+1}} \qquad (3.13b)$$

in which T_ℓ is the kinetic energy-angular momentum radial operator given by

$$T_\ell(r) = -\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{\ell(\ell+1)}{r^2} \quad ; \qquad (3.14)$$

and A is a numerical angular factor[12] which can be expressed as

$$A(\lambda, L_i, \ell_i, L_j, \ell_j, L) = (-1)^{\ell_j + L_i - L}\,[(2\ell_i+1)(2\ell_j+1)(2L_i+1)(2L_j+1)]^{\frac{1}{2}} \\ \times \begin{Bmatrix} L & \ell_i & L_i \\ \lambda & \ell_j & L_j \end{Bmatrix} \begin{pmatrix} \ell_j & \lambda & L_i \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_j & \lambda & \ell_i \\ 0 & 0 & 0 \end{pmatrix} . \qquad (3.15)$$

The {....} is a 6-j symbol, while (....) is a 3-j symbol. The index λ lies in the interval.

$$\text{Maximum } (|L_i-\ell_j|,|L_j-\ell_i|) \leq \lambda < \text{Minimum } (L_j+\ell_i, L_i+\ell_j). \tag{3.16}$$

The functional now reduces to

$$I_{ab} = \sum_{i,j=1}^{n_o} \iint dr_1 dr_2 \; r_1^2 \, r_2^2 \; [R_i(r_1) \; G_{ia}(r_2) \; H_D^{ij}(r_1,r_2) \pm R_i(r_2) \; G_{ia}(r_1) \; H_x^{ij}(r_1,r_2)] \; R_j(r_1) \; G_{jb}(r_2) \tag{3.17}$$

where, as defined in Eq. (2.14),

$$G_{ia}(r) = \sum_{s=1}^{2} (\alpha_s)_{ia} \; f_s(k_i,r) + \sum_{\mu=1}^{n_c} C_{ia,\mu} \; \eta_\mu^{(i)}(r)$$

$$G_{jb}(r) = \sum_{s=1}^{2} (\alpha_t)_{jb} \; f_t(k_j,r) + \sum_{\nu=1}^{n_c} C_{jb,\nu} \; \eta_\nu^{(j)}(r) \tag{3.18}$$

Substituting in Eq. (3.17), we reduce the three principal types of matrix elements, defined in Section II.D, to the following expressions:

(i) the bound-bound matrix elements

$$B_{\mu\nu}^{ij} = \int_0^\infty \int_0^\infty dr_1 dr_2 \; r_1^2 r_2^2 \; [R_i(r_1) \; \eta_\mu^{(i)}(r_2) \; H_D^{ij}(r_1,r_2) \pm R_i(r_2) \; \eta_\mu^{(i)}(r_1) \; H_x^{ij}(r_1,r_2)] \; R_j(r_1) \; \eta_\mu^{(j)}(r_2) \tag{3.19}$$

which involve bound Slater orbitals only.

(ii) the bound-free matrix elements

$$M_{\mu t}^{ij} = \int_0^\infty\int_0^\infty dr_1 dr_2\ r_1^2 r_2^2\ [R_i(r_1)\ \eta_\mu^{(i)}(r_2)\ H_D^{ij}(r_1,r_2) \pm R_i(r_2)\ \eta_\mu^{(i)}(r_1)\ H_x^{ij}(r_1,r_2)]\ R_j(r_1)\ f_t(k_j,r_2) \tag{3.20}$$

which involve Slater orbitals and one free long range function.

(iii) the free-free matrix elements

$$F_{st}^{ij} = \int_0^\infty\int_0^\infty dr_1 dr_2\ r_1^2 r_2^2\ [R_i(r_1)\ f_s(k_i,r_2)\ H_D^{ij}(r_1,r_2) \pm R_i(r_2)\ f_s(k_i,r_2)\ H_x^{ij}(r_1,r_2)]\ R_j(r_1)\ f_t(k_j,r_2) \tag{3.21}$$

which involve Slater orbitals and two free long range functions.

These expressions, (3.19) through (3.21), can be further reduced by considering the properties of the target wave functions, specifically, their orthogonality

$$\int_0^\infty dr\ r^2\ R_j(r)\ R_{j'}(r) = \delta_{jj'}, \tag{3.22}$$

and the condition they satisfy (refer to Eq. (2.6))

$$\int_0^\infty dr\ r^2\ R_{j'}(r)\ [T_{\ell_j} - 2\ Z/r - E_j\ \delta_{jj'}]\ R_j(r) = 0. \tag{3.23}$$

which holds for both real eigenstates and pseudostates.

Combining Eqs. (3.22), (3.23), and (3.19-21), the direct matrix elements reduce to

$$d_{B_{\mu\nu}}^{ij} = \delta_{ij}\,\delta_{\ell_i\ell_j}\,\delta_{L_iL_j}\int_0^\infty dr_2\, r_2^2\,\eta_\mu^{(i)}(r_2)\,[T_{\ell_j} - 2\,Z/r_2 - k_j^2]\,\eta_\nu^{(j)}(r_2) + 2\sum_\lambda A(\lambda,L_i,\ell_i,L_j,\ell_j,L)\iint_{00}^{\infty\infty} dr_1dr_2\, r_1^2r_2^2\,R_i(r_1)\,\eta_\mu^{(i)}(r_2)\,\frac{r_<^\lambda}{r_>^{\lambda+1}}\,R_j(r_1)\,\eta_\nu^{(j)}(r_2)\;; \tag{3.24}$$

$$d_{M_{\mu t}}^{ij} = \delta_{ij}\,\delta_{\ell_i\ell_j}\,\delta_{L_iL_j}\int_0^\infty dr_2\, r_2^2\,f_t(k_j,r_2)\,[T_{\ell_j} - 2\,Z/r_2 - k_j^2]\,\eta_\mu^{(i)}(r_2) + 2\sum_\lambda A(\lambda,L_i,\ell_i,L_j,\ell_j,L)\iint_{00}^{\infty\infty} dr_1dr_2\, r_1^2r_2^2\,R_i(r_1)\,\eta_\mu(r_2)\,\frac{r_<^\lambda}{r_>^{\lambda+1}}\,R_j(r_1)\,f_t(k_j,r_2)\;; \tag{3.25}$$

and

$$d_{F_{s_t}}^{ij} = \delta_{ij}\,\delta_{\ell_i\ell_j}\,\delta_{L_iL_j}\int_0^\infty dr_2\, r_2^2\,f_s(k_i,r_2)\,[T_{\ell_j} - 2\,Z/r_2 - k_j^2]\,f_t(k_j,r_2) + 2\sum_\lambda A(\lambda,L_i,\ell_i,L_j,\ell_j,L)\iint_{00}^{\infty\infty} dr_1dr_2\, r_1^2r_2^2\,R_i(r_1)\,f_s(k_i,r_2)\,\frac{r_<^\lambda}{r_>^{\lambda+1}}\,R_j(r_1)\,f_s(k_j,r_2) \tag{3.26}$$

In order to express the matrix elements (direct or exchange) in terms of some specific integrals, we will use the representation of the target functions as sums of Slater orbitals (refer to Section II.C)

$$\begin{cases} R_i(r) = \sum_{m_i=1}^{N_i} C^i_{J_i,m_i}\, r^{n_{m_i}}\, e^{-z_{m_i}r} \\ R_j(r) = \sum_{m_j=1}^{N_j} C^i_{J_j,m_j}\, r^{n_{m_j}}\, e^{-z_{m_j}r} \end{cases} \tag{3.27}$$

in which N_i and N_j denote the number of elements in the i-th and j-th pseudobases, respectively, and J_i and J_j are the angular momenta L_i and L_j plus unity. We note here that the set of exponents (z_{m_k}), expansion coefficients ($C^k_{J_k,m_k}$), and energies (E_k) of the k-th target function, have a definite scaling behavior with the nuclear charge Z (Table I). The short range basis elements which appear in the expansion of $G_{ka}(r)$ are written as

$$\eta^{(i)}_\alpha(r) = r^{\ell_\alpha} e^{-\zeta_\alpha r} , \qquad (3.28a)$$

and the long range functions as

$$f_p(k,r) = r^{-n} (1-e^{-\gamma r})^J U_p(\ell,kr) \qquad (3.28b)$$

in which Up stands for the regular (p=1) and the irregular (p=2) Coulomb functions, and n = 1, 2, ...

This particular form of f_p has been introduced in order to have the flexibility of adding energy dependent (properly regularized) Coulomb functions with r^{-n} dependence ($n \geq 2$) to the short range basics above the n = 2 threshold.[39] We found, however, that such functions were not needed in order to achieve acceptable accuracy. The long range off diagonal dipole couplings between degenerate channels are less significant for high Z ions. In this case an expansion in Slater type orbitals is capable of describing the scattering wave function near the ion.

We now combine Eqs. (3.27) and (3.28) with the expressions (3.24) - (3.26) and rewrite the direct matrix elements as

(i) The direct bound-bound elements

$$d_{B_{\mu\nu}}^{ij} = \delta_{ij}\,\delta_{\ell_i\ell_j}\,\delta_{L_iL_j}\int_0^\infty dr_2\, r_2^2\,\eta_\mu^{(i)}(r_2)\,[T_{\ell_j} - 2Z/r_2 - k_j^2]\,\eta_\nu^{(j)}(r_2) + 2\sum_\lambda A(\lambda,L_i,\ell_i,L_j,\ell_j,L) \sum_{m_i=1}^{N_i}\sum_{m_j=1}^{N_j} C^i_{J_i,m_i}\,C^i_{J_j,m_j} \int_0^\infty\int_0^\infty dr_1dr_2\, r_1^2r_2^2\,(r_2^{\ell_\mu} e^{-\zeta_\mu r_2})(r_1^{n_{m_i}} e^{-z_{m_i}r_1})\,\frac{r_<^\lambda}{r_>^{\lambda+1}}\,(r_2^{\ell_\nu} e^{-\zeta_\nu r_2})(r_1^{n_{m_j}} e^{-z_{m_i}r_1}) \qquad (3.29)$$

which involve two bound-bound type integrals, and maybe expressed as

$$d_{B_{\mu\nu}}^{ij} = \delta_{ij}\,\delta_{\ell_i\ell_j}\,\delta_{L_iL_j}\,D_{\mu\nu}^{ij}(\ell_\mu,\zeta_\mu;\ell_\nu,\zeta_\nu;\ell_j,Z,k_j) + 2\sum_\lambda A(\lambda,L_i,\ell_i,L_j,\ell_j,L) \sum_{m_i=1}^{N_i}\sum_{m_j=1}^{N_j} C^i_{J_i,m_j}\,C^j_{J_j,m_j}\, N_{\mu\nu}^{ij}(\ell_\mu,\zeta_\mu,n_{m_i},z_{m_i};\lambda;\ell_\nu,\zeta_\nu,n_{m_j},z_{m_j})\,. \qquad (3.30)$$

The computation of the D and N type integrals give, respectively, the kinetic energy and direct potential contribution to the direct bound-bound matrix elements.

The radial matrix elements of the direct interaction potential are defined by

$$V_\lambda^{m_i m_j}(r_2) = \int_0^\infty dr_1\, r_1^2\, (r_1^{n_{m_i}} e^{-z_{m_i} r_1}) \frac{r_<^\lambda}{r_>^{\lambda+1}} (r_1^{n_{m_i}} e^{-z_{m_i} r_1}) \quad (3.31)$$

The N type integrals contain these elements (which will be explicitly evaluated in Appendix B) and thus may be rewritten as

$$N_{\mu\nu}^{ij}(\lambda) = \int_0^\infty dr_2\, r_2^2\, (r_2^{\ell_\mu} e^{-\zeta_\mu r_2})\, V_\lambda^{m_i m_j}(r_2)\, (r_2^{\ell_\nu} e^{-\zeta_\nu r_2}) \quad (3.32)$$

(For simplicity of notations we will drop the arguments of the integrals, leaving only the outstanding ones).

(ii) The direct bound free elements

$$\begin{aligned} d_{M_{\mu t}^{ij}} = {} & \delta_{ij}\delta_{\ell_i\ell_j}\delta_{L_iL_j} \int_0^\infty dr_2\, r_2^2\, (r_2^{\ell_\mu} e^{-\zeta_\mu r_2}) \left[T_{\ell_j} - 2Z/r_2 - k_j^2\right] f_t(k_j, r_2) \\ & + 2 \sum_\lambda A(\lambda, L_i, \ell_i, L_j, \ell_j, L) \sum_{m_i=1}^{N_i} \sum_{m_j=1}^{N_j} C^i_{J_i, m_i} C^j_{J_i, m_j} \int\int_{00}^{\infty\infty} dr_1 dr_2\, r_1^2\, r_2^2\, (r_2^{\ell_\mu} e^{-\zeta_\mu r_2}) \\ & (r_1^{n_{m_i}} e^{-z_{m_i} r_1}) \frac{r_<^\lambda}{r_>^{\lambda+1}} (r_1^{n_{m_i}} e^{-z_{m_i} r_1})\, f_t(k_j, r_2) \end{aligned} \quad (3.33)$$

which involve 2 bound-free type integrals. The B type integral which gives the kinetic energy contribution, and the X type integral which gives the direct potential contribution to these particular matrix elements. Eq. (3.33) now reads

$$d_{M_{\mu t}^{ij}} = \delta_{ij}\delta_{\ell\ \ell}\delta_{L_iL_j}\ B_{\mu t}^{ij}\ (\ell_2,j_2,\gamma_2;\ell_j,k_j,Z;\ell_\mu,\zeta_\mu) + 2\ \sum_{\lambda}$$

$$A(\lambda,L_i,\ell_i,L_j,\ell_j,L) \quad \sum_{m_k=1}^{N_i}\ \sum_{m_j=1}^{N_j}\ C^i_{J_i,m_i}\ C^j_{J_j,m_j}$$

$$X^{ij}_{\mu t}(\ell_\mu,\zeta_\mu,n_{m_i},z_{m_i};\lambda;\ell_2,j_2,\gamma_2,\ell_j,k_j,n_{m_j},z_{m_j}) \tag{3.34}$$

in which the arguments $\{\ell_2,j_2,\gamma_2\}$ characterize the free function

$$f_t(k_j,r_2) = r_2^{-\ell_2}\ (1-e^{-\gamma_2 r_2})^{j_2}\ U_t(\ell_j,k_j,r_2) \tag{3.35}$$

(iii) The direct free-free elements

$$d_{F_{s_t}^{ij}} = \delta_{ij}\delta_{\ell_i\ell_j}\delta_{L_iL_j}\ A^{ij}_{s_t}(\ell_1,j_1,\gamma_1,\ell_i,k_i;\ell_2,j_2,\gamma_2,\ell_j,k_j;Z)$$

$$+ 2\ \sum_{\lambda}\ A(\lambda,L_i,\ell_i,L_j,\ell_j,L) \quad \sum_{m_i=1}^{N_i}\ \sum_{m_j=1}^{N_j}\ C^i_{J_i,m_i}\ C^i_{J_j,m_j}$$

$$I^{ij}_{s_t}(n_{m_i},z_{m_i},\ell_1,j_1,\gamma_1,\ell_i,k_i;\lambda;n_{m_j},z_{m_j},\ell_2,j_2,\gamma_2,\ell_j,k_j) \tag{3.36}$$

in which the free-free type integrals

$$A^{ij}_{s_t} = \int_0^\infty dr_2\ r_2^2\ f_s(k_i,r_2))\ [T_{\ell_j} - 2(Z-1)/r_2 - k_j^2]\ f_t(k_j,r_2) \tag{3.37}$$

and

$$I^{ij}_{s_t}(\lambda) = \int_0^\infty dr_2\ r_2^2\ f_s(k_i,r_2)\ U^\lambda_{m_im_j}(r_2)\ f_t(k_j,r_2) \tag{3.38}$$

respectively evaluate the kinetic energy contribution and the potential energy contribution to direct free-free

matrix elements.

The modified potential matrix elements, $U^{\lambda}_{m_i m_j}$, defined by

$$U^{\lambda}_{m_i m_j}(r) = V_{\lambda}^{m_i m_j}(r) - \frac{\alpha_{m_i m_j}}{r^{\lambda+1}} \delta_{ij} \delta_{\ell_i \ell_j} \delta_{L_i L_j} \tag{3.39}$$

are conveniently introduced in order to avoid numerical difficulties which arise in the case $\lambda=0$. These difficulties are associated with the asymptotic behavior of the direct potential elements

$$V_{\lambda}^{m_i m_j}(r) \xrightarrow[r\to\infty]{} \frac{\alpha_{m_i m_j}}{r^{\lambda+1}} \tag{3.40}$$

the coefficients α are evaluated in Appendix B. We also note here that the parameters ℓ_1, j_1 and γ_1 are associated with the free function

$$f_s(k_i, r_2) = r_2^{-\ell_1} (1-e^{-\gamma_1 r_2})^{j_1} U_s(\ell_i, k_i r_2) \ . \tag{3.41}$$

In a similar manner, exchange matrix elements can be expressed in terms of some specific integrals. In this case, we have

(i) The exchange bound-bound elements

$$x_{B}{}^{ij}_{\mu\nu} = \int_0^{\infty}\int_0^{\infty} dr_1 dr_2 \ r_1^2 r_2^2 \ R_i(r_2) \ \eta_{\mu}^{(i)}(r_1) \ [\delta_{\ell_i L_j} \ \delta_{\ell_i L_i} (T_{\ell_i} + T_{L_i} - 2Z/r_1 - 2 \ Z/r_2 - E) + 2 \sum_{2} A(\lambda, \ell_i, L_i, L_j, \ell_j, L) \frac{r_<^{\lambda}}{r_>^{\lambda+1}}] \ R_j(r_1) \ \eta_{\nu}^{(j)}(r_2) \tag{3.42}$$

which, using the expansions (3.27) and (3.28), can be explicitly written as

$$x_{B_{\mu\nu}}^{ij} = \sum_{m_i=1}^{N_i} \sum_{m_j=1}^{N_j} C^i_{J_i,m_i} C^j_{J_j,m_j} \{\delta_{\ell_i L_j} \delta_{\ell_j L_i} \int_0^\infty\int_0^\infty dr_1 dr_2$$

$$(r_2^{n_{m_i}} e^{-z_{m_i} r_2}) (r_1^{\ell_\mu} e^{-\zeta_\mu r_1}) \quad [T_{\ell_i} + T_{\ell_j} - 2\,Z/r_2 - E]$$

$$(r_1^{n_{m_j}} e^{-z_{m_j} r_1}) (r_2^{\ell_\nu} e^{-\zeta_\nu r_2}) + 2 \sum_\lambda A(\lambda, \ell_i, L_i, L_j, \ell_j, L)$$

$$\int_0^\infty\int_0^\infty dr_1 dr_2\, r_1^2 r_2^2 (r_2^{n_{m_i}} e^{-\zeta_{m_i} r_2}) (r_2^{\ell_\nu} e^{-\zeta_\nu r_2})$$

$$\frac{r_<^\lambda}{r_>^{\lambda+1}} (r_1^{n_{m_j}} e^{-\zeta_{m_j} r_1}) (r_1^{\ell_\mu} e^{-\zeta_\mu r_1})\} \qquad (3.43)$$

in which the second integral is an N type integral defined above, and the first is another bound-bound type integral, $P_{\mu\nu}^{ij}$, whose evaluation gives the single particle Hamiltonian contribution. Eq. (3.43) reduces to

$$x_{B_{\mu\nu}}^{ij} = \sum_{m_i=1}^{N_i} \sum_{m_j=1}^{N_j} C^i_{J_i,m_i} C^j_{J_i,m_j} \{\delta_{\ell_i L_j} \delta_{\ell_j L_i} P_{\mu\nu}^{ij}(\ell_\mu, \zeta_\mu, n_{m_i},$$

$$z_{m_i}; \ell_\nu, \zeta_\nu, n_{m_j}, z_{m_j}, \ell_i, \ell_j, Z, E) + 2 \sum_\lambda A(\lambda, \ell_i, L_i, L_j, \ell_j, L)$$

$$N_{\mu\nu}^{ij}(n_{m_i}, z_{m_i}, \ell_\mu, \zeta_\mu; \lambda; \ell_\nu, \zeta_\nu, n_{m_j}, z_{m_j})\} \qquad (3.44)$$

(ii) Exchange bound-free elements

Combining Eqs. (3.13), (3.20), (3.27), and (3.28), we can express these elements as

$$x_{M_{\mu t}}^{ij} = \sum_{m_i=1}^{N_i} \sum_{m_j=1}^{N_j} C_{j_i,m_i}^{i} C_{J_i,m_j}^{j} \{\delta_{\ell_i L_i} \delta_{\ell_j L_i} G_{\mu t}^{ij} (n_{m_i}, z_{m_i}, \ell_\mu, \zeta_\mu; n_{m_j}, z_{m_j}, \ell_2, j_2, \gamma_2; \ell_i, \ell_j, Z, E) + 2 \sum_{\lambda} A(\lambda, \ell_i, L_i, L_j, \ell_j, L) X_{\mu t}^{ij} (n_{m_i}, z_{m_i}, \ell_\mu, \zeta_\mu; \lambda; \ell_2, j_2, \gamma_2, \ell_j, k_j, n_{m_j}, z_{m_j})\} \quad (3.45)$$

in which the bound-free type integrals

$$G_{\mu t}^{ij} = \int_0^\infty \int_0^\infty dr_1 dr_2 \, r_1^2 r_2^2 \, (r_1^{\ell_\mu} e^{-\zeta_\mu r_1}) (r_2^{n_{m_i}} e^{-z_{m_i} r_2}) \, [T_{\ell_i} + T_{\ell_j} - 2 Z/r_1 - 2 Z/r_2 - E] \, (r_1^{n_{m_j}} e^{-z_{m_j} r_1}) \, f_t(k_j, r_2) \quad (3.46)$$

evaluate the single particle Hamiltonian contribution. The second integral (X-type) has already been defined above; its evaluation yields, the direct potential contribution.

(iii) Exchange free-free elements

Likewise, we introduce 2 free-free type integrals. The ε integral defined by

$$\varepsilon^{ij}_{s_t} = \int_0^\infty\int_0^\infty dr_1 dr_2\, r_1^2 r_2^2\, f_s(k_i,r_1)\,(r_2^{n_{m_i}} e^{-z_{m_i} r_2})\,[T_{\ell_i} + T_{\ell_j} - 2Z/r_1 - 2Z/r_2 - E]\, f_t(k_j,r_2)\,(r_1^{n_{m_j}} e^{-z_{m_j} r_1}) \quad (3.47)$$

and the H-integral defined by

$$H^{ij}_{s_t} = \int_0^\infty dr_1\, r_1^2\, f_s(k_i,r_1)\,(r_1^{n_{m_j}} e^{-z_{m_j} r_1}) \int_0^\infty dr_2\, r_1^2\, f_t(k_j,r_2)\, \frac{r_<^\lambda}{r_>^{\lambda+1}}\,(r_2^{n_{m_i}} e^{-z_{m_i} r_2}) \quad (3.48)$$

The first type evaluates the single particle Hamiltonian contribution, while the second evaluates the interaction potential contribution to the exchange free-free elements which can now be expressed as

$$x_{F^{ij}_{s_t}} = \sum_{m_i=1}^{N_i}\sum_{m_j=1}^{N_j} C^i_{J_i,m_i}\, C^j_{J_j,m_j}\,\{\delta_{\ell_i L_j}\,\delta_{\ell_j L_i}\,\varepsilon^{ij}_{s_t}(\ell,j_1,\gamma_1,\ell_i,k_i,n_{m_i},z_{m_i};\ell_2,j_2,\gamma_2,\ell_j,k_j,n_{m_j},z_{m_j};Z,E) + 2\sum_\lambda A(\lambda,\ell_i,L_i,L_j,\ell_j,L)\, H^{ij}_{s_t}(n_{m_i},z_{m_i},\ell_1,j_1,\gamma_1,\ell_i,k_i;\lambda;n_{m_j},z_{m_j},\ell_2,j_2,\gamma_2,\ell_j,k_j)\}\,. \quad (3.49)$$

In conclusion, we remark that the evaluation of the bound-free type integrals can be simplified by letting the differential operators act on the short range functions rather than on the long range function. We also note that the exchange free-free integrals basically involve the pro-

duct of 2 bound-free integrals.

The problem of evaluating the 3 main types of matrices, is reduced to the evaluation of a set of specific integrals which will be our concern in the next section.

B. Evaluation of Specific Integrals

These integrals are classified into 3 main categories: bound-bound, bound-free and free-free. In representing these integrals, the lower indices specify the particular matrix elements, while the upper indices stand for the channels in interaction.

1. Bound-bound type integrals

Analytic expressions can be obtained for all these integrals which involve only Slater type orbitals.

(i) D Integral

This integral is defined by

$$D_{nm}^{ij}(n,a;m,b,\ell,p,Z) = \int_0^\infty dr\, r^2 (r^n e^{-ar}) \, [T_\ell - 2\,Z/r - p^2] \, (r^m e^{-br}) \qquad (3.50)$$

in which

$$T_\ell = -\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr}\right) + \frac{\ell(\ell+1)}{r^2}$$

Applying the kinetic energy operator on $(r^m e^{-br})$, we get

$$\left[-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\right]\left(r^m e^{-br}\right) = \left[-b^2 + \frac{2(m+1)b}{r} - \frac{m(m+1)}{r^2}\right] \left(r^m e^{-br}\right) ;$$

then

$$\left[T_\ell - 2Z/r - p^2\right]\left(r^m e^{-br}\right) = \left[b_1 + b_2/r + b_3/r^2\right]\left(r^m e^{-br}\right) \tag{3.51}$$

in which

$$b_1 = -(b^2 + p^2) \quad ,$$

$$b_2 = 2[(m+1) - Z] \quad , \tag{3.52}$$

and

$$b_3 = \ell(\ell+1) - m(m+1) \quad .$$

The integral can now be written as

$$D^{ij}_{nm} = \int_0^\infty dr\, r^2\, r^n\, e^{-ar}\left[b_1 + b_2/r + b_3/r^2\right] r^m\, e^{-br} \quad ,$$

which is the sum of analytic integrals of the type

$$In(\alpha) = \int_0^\infty dx\, x^n\, e^{-\alpha x} = n!\ \alpha^{-(n+1)} \quad ; \tag{3.53}$$

that is

$$D^{ij}_{nm} = b_1 \frac{(m+n+2)!}{(a+b)^{m+n+3}} + b_2 \frac{(m+n+1)!}{(a+b)^{m+n+2}} + b_3 \frac{(m+n)!}{(a+b)^{m+n+1}}$$

or more conviently, written as

$$D^{ij}_{nm} = \frac{(m+n)!}{(a+b)^{m+n+3}}\{b_1(m+n+1)(m+n+2) + (a+b)\left[b_2(m+n+1) + b_3(a+b)\right]\} \tag{3.54}$$

with b_i $(i = 1, 3)$ given by Eq. (3.52)

(ii) P Integral

This bound-bound type integral is given by

$$P^{ij}_{nn'}(n,a,m,b;n',a',m',b';\ell',\ell',Z,E) = \int_0^\infty dx\ (x^n e^{-ax})$$

$$x^2\ (x^{m'} e^{-b'x}) \int_0^\infty dr\ r^2\ (r^m e^{-br})\ [T_{\ell'} - 2Z/r - E]$$

$$(r^{n'} e^{-a'r}) + \int_0^\infty dx\ x^2\ (x^m e^{-bx})\ (x^{n'} e^{-a'x}) \int_0^\infty dr\ r^2$$

$$(r^n e^{-ar})\ [T_\ell - 2Z/r]\ (r^{m'} e^{-b'r})\ . \qquad (3.55)$$

The 2 integrals

$$D_1 = \int_0^\infty dr\ r^2\ r^m\ e^{-br}\ [T_{\ell'} - 2Z/r - E]\ r^{n'}\ e^{-a'r}$$

and

$$D_2 = \int_0^\infty dr\ r^2\ r^n\ e^{-ar}\ [T_\ell - 2Z/r]\ r^{m'}\ e^{-b'r}$$

are D type integrals which, using Eq. (3.54), can be expressed as

$$D_1 = \frac{(m+n')!}{(a'+b)^{m+n'+3}} \{a_1\ (m+n'+1)(m+n'+2) + (a' + b)$$

$$[a_2\ (m+n'+1) + a_3(a'+b)]\}$$

in which $a_1 = -\ (a'^2 + E)$,

$a_2 = 2\ [(n' + 1)\ a' - Z]$, (3.56)

and

$a_3 = \ell'(\ell' + 1) - n'(n' + 1)$;

and

$$D_2 = \frac{(n+m')!}{(a+b')^{n+m'+3}} \{b_1(n+m'+1)(m'+n+2) + (a+b')\ [b_2(n+m'+1)$$

$$+ b_3\ (a+b')]\}$$

in which

$$b_1 = -b'^2 \quad ,$$

$$b_2 = 2[(m'+1)b' - Z] \quad ,$$

and (3.57)

$$b_3 = \ell(\ell + 1) - m'(m'+1) \quad .$$

Combining (3.55), (3.56), and (3.57), we get

$$P^{ij}_{nn'} = \frac{(n+m'+2)!}{(a+b')^{n+m'+3}} \{\frac{(m+n')!}{(a'+b)^{m+n'+3}}[a_1 \ (m+n'+1)(m+n'+2)$$

$$+ (a'+b) \{a_2 \ (m+n'+1) + a_3(a' + b)\}]\}$$

$$+ \frac{(m+n'+2)!}{(a'+b)^{m+n'+3}} \{\frac{(n+m')!}{(a+b')^{n+m'+3}} [b_1 \ (n+m'+1)$$

$$(n+m'+2) + (b'+a) \{b_2 \ (n+m'+1) + (b'+a) \ b_3\}]\}$$

(3.58)

which could be written in a more convenient form:

$$P^{ij}_{nn'} = P_o\{(n+m'+2)(n+m'+1) \ [a_1(m+n'+1)(m+n'+2) + (a'+b)$$

$$\{a_2(m+n'+1) + a_3(a'+b)\}] + (n'+m+2)(n'+m+1)$$

$$[b_2(n+m'+1)(n+m'+2) + (b'+a) \ \{b_2(n+m'+1)$$

$$+ b_3 \ (a+b')\}]\} \qquad (3.59)$$

where

$$P_o = \frac{(m+n')! \ (n+m')!}{(a'+b)^{m+n'+3} \ (a+b')^{n+m'+3}}$$

and a_i (i = 1, 3) and b_j (i = 1, 3) are given in Eqs. (3.56) and (3.57).

(iii) N Integral

This integral is defined by

$$N^{ij}_{nn'}\ (n,a,m,b;\ell;n',a',m',b;) = \int_0^\infty dr\ r^2\ (r^n\ e^{-ar})\,(r^{n'}\ e^{-a'r})$$

$$V_\ell^{mm'}\ (m,b;m',b';r) \qquad (3.60)$$

in which $V_\ell^{mm'}(r) = \int_0^\infty dx\ x^2\ (x^m\ e^{-bx})\ \frac{x_<^\ell}{x_>^{\ell+1}}\ (x^{m'}\ e^{-b'x})$

where $x_<$ is the lesser and $x_>$ is the greater of $\{x,r\}$.

The V integral is evaluated in details in Appendix B, it is given by the expression

$$V_\ell^{mm'}(r) = \frac{(m+m'+\ell+2)!}{(b+b')^{m+m'+\ell+3}\ r^{\ell+1}}\ \{1 - e^{-(b+b')r} \sum_{\nu=0}^{m+m'+\ell+1}$$

$$h(m,m';\ell,\nu;b,b')r^\nu\} \qquad (3.61)$$

in which the function h is given by

$$h(m,m';\ell,\nu,b,b') = \frac{1}{\nu!} - [\frac{(m+m'+1-\ell)!}{(m+m'+\ell+2)!\ (\nu-2\ -1)!}]\ (b+b')^\nu. \qquad (3.62)$$

Combining (3.60) and (3.61), the N integral can be written as:

$$N^{ij}_{nn'} = \frac{(m+m'+\ell+2)!}{(b+b')^{m+m'+\ell+3}}\ \{\int_0^\infty dr\ r^2\ (r^n\ e^{-ar})\ r^{-\ell-1}\ (r^{n'}\ e^{-a'r})$$

$$- \sum_{\nu=0}^{m+m'+\ell+1} h(m,m';\ell,\nu;b,b') \int_0^\infty dr\ r^2\ (r^n\ e^{-ar})$$

$$r^{\nu-\ell-1}\ e^{-(b+b')r}\ (r^{n'}e^{-a'r})\}. \qquad (3.63)$$

The integral now involves the simple integrals $I_n(\alpha)$, and thus can be expressed as

$$N^{ij}_{nn'} = \frac{(m+m'+\ell+2)!}{(b+b')^{m+m'+\ell+3}} \left\{ \frac{(n+n'+1-\ell)!}{(a+a')^{n+n'+2-\ell}} - \sum_{\nu=0}^{m+m'+\ell+1} h(m,m';\ell,\nu;b,b') \frac{(n+n'+\nu+1-\ell)!}{(a+a'+b+b')^{n+n'+\nu+2-\ell}} \right\} \quad (3.64)$$

2. Bound-free type integrals

Analytic expressions are obtained for bound-free integrals which involve the regular Coulomb function; otherwise numerical integrations are performed.

(i) B Integral

This integral is defined by

$$B^{ij}_{ms}(n,J_s,\gamma;\ell,p,Z;m,a) = \int_0^\infty dr\, r^2\, f_s(n,J_s,\gamma;\ell,pr) \left[T_\ell - 2Z/r - p^2\right](r^m e^{-ar}) \quad (3.65)$$

in which

$$f_1 = r^{-n}(1 - e^{-\gamma r})^{J_1} F_\ell(pr), \quad J_1 = n - 1$$
$$f_2 = r^{-n}(1 - e^{-\gamma r})^{J_2} G_\ell(pr), \quad J_2 = 2\ell + n . \quad (3.66)$$

The parameter n is an integer greater than or equal to one, and F_ℓ and G_ℓ are, respectively, the regular and irregular Coulomb function denoted by $U_S(\ell,pr)$.

Referring to Eq. (3.51), we have

$$[T - 2Z/r - p^2](r^m e^{-ar}) = \left[-(a^2+p^2) + \frac{2\{(m+1)a - Z\}}{r} + \frac{\ell(\ell+1) - m(m+1)}{r^2}\right](r^m e^{-ar}) ,$$

which we will conveniently rearrange in the following form

$$[T_\ell - 2\,Z/r - p^2](r^m\, e^{-ar}) = \{[a_1 + a_2/r + a_3/r^2] - 2/r\}\,(r^m\, e^{-ar}) \qquad (3.67)$$

in which

$$a_1 = -(a^2 + p^2) \quad ,$$
$$a_2 = 2[(m+1)\,a-(Z-1)] \quad , \qquad (3.68)$$

and

$$a_3 = \ell(\ell + 1) - m(m + 1) \quad .$$

For the case s=1 (involving the regular Coulomb function), the integral can be expressed as a sum of T type integrals defined by

$$T_s(n,a,J_s,\gamma,\ell,p) = \int_0^\infty dr\; r^n\, e^{-ar}\,(1-e^{-\gamma r})^{J_s}\, U_s(\ell,pr). \qquad (3.69)$$

that is

$$B_{ms}^{ij} = \{a_1\, T_s(m+2-n,a,J_s,\gamma;\ell,p) + a_2\, T_s(m+1-n,a,J_s,\gamma;\ell,p) + a_3\, T_s(m-n,a,J_s,\gamma;\ell,p)\} - 2\, T_s(m+1-n,a,J_s,\gamma;\ell,p) \qquad (3.70)$$

with a_i (i = 1, 3) given in Eq. (3.68). We note here that the T type integrals will be evaluated explicitly in Appendix C.

The expression given above, reduces to a single T type integral in the special case n = 1, J_s = 0. In fact, the symmetry of bound-free integrals allows the differential

operator to act on the free function. This yields

$$[T_\ell - \frac{2(Z-1)}{r} - p^2] \quad \frac{U_s(\ell,pr)}{r} = 0$$

which is the Coulomb differential equation (3.70) reduces to

$$B^{ij}_{m_1} = -2\ T_2\ (m+1-n,a,J_1,\gamma;\ell,p). \qquad (3.71)$$

On the other hand, for the case "s=2" which involves the irregular Coulomb function, we write

$$B^{ij}_{ms} = \int_0^\infty dr\ r^{m+2-n}\ e^{-ar}\ (1-e^{-\gamma r})^{J_s}\ [a_1+(a_2-2)/r + a_3/r_2]$$
$$U_s(\ell,pr) \qquad (3.72)$$

and evaluate the integral numerically (refer to Appendix C).

(ii) G Integral

This bound-free type integral is given by

$$G^{ij}_{ns}(n,a,m,b;n',a',\nu,\gamma,J_s,\ell,\ell',p,Z,E) = \int_0^\infty dr\ r^2\ (r^m\ e^{-br})$$
$$(r^{n'}\ e^{-a'r}) \int_0^\infty dr\ r^2\ (r^n\ e^{-ar}) \quad [T_\ell - 2\ Z/r - E]\ f_s$$
$$(\nu,J_s,\gamma;\ell,pr) + \int_0^\infty dr\ r^2\ (r^n\ e^{-ar})\ f_s\ (\nu,J_s,\gamma;\ell,pr)$$
$$\int_0^\infty dr\ r^2\ (r^m\ e^{-br})\ [T_{\ell'} - 2\ Z/r]\ (r^{n'}\ e^{-a'r}) \qquad (3.73)$$

with f_s as defined in eq. (3.66).

The differential operators may be made to act on the short range functions, which enables us to use Eq. (3.54) and the integrals $I_n(\alpha)$, and thus reduce the integral to a simpler form. In fact we have

$$g_1 = \int_0^\infty dr\ r^2\ (r^m\ e^{-br})\ (r^{n'}\ e^{-a'r}) = \frac{(m+n'+2)!}{(a'+b)^{m+n'+3}}\ , \tag{3.74}$$

and

$$g_2 = \int_0^\infty dr\ r^2\ (r^m\ e^{-br})\ [T_{\ell'} - 2Z/r]\ (r^{n'}\ e^{-a'r})$$

$$= \frac{(m+n')!}{(a'+b)^{m+n'+3}} \{a_2'\ (m+n'+1)\ (m+n'+2) + (a'+b)$$

$$[a_2'(m+n'+1) + a_3'(a'+b)]\} \tag{3.75}$$

in which $a_1' = -a'^2$,

$$a_2' = 2\ [(n'+1)\ a'-Z]\ , \tag{3.76}$$

and $a_3' = \ell'(\ell'+1) - n'(n'+1)$

Besides, using Eq. (3.51), we get

$$[T_\ell - 2\ Z/r - E]\ (r^n\ e^{-ar}) = [a_1+a_2/r+a_3/r^2]\ (r^n\ e^{-ar}) \tag{3.77}$$

in which

$$a_1 = -\ (a^2 + E)\ , \qquad a_2 = 2\ [(n+1)\ a-Z]\ , \tag{3.78}$$

and

$$a_3 = \ell(\ell+1) - n(n+1)\ .$$

Combining Eqs. (3.73) through (3.78), the integral reduces to

$$G_{ns}^{ij} = g_1 \int_0^\infty dr\ r^2\ r^{-\nu}(1-e^{-\gamma r})^{J_s}\ U_s(\ell,pr)\ [a_2+a_2/r+a_3/r^2]$$

$$(r^n\ e^{-ar}) + g_2 \int_0^\infty dr\ r^2\ r^{-\nu}\ (1-e^{-\gamma r})^{J_s}\ U_s(\ell,pr)$$

$$(r^n\ r^{-ar})\ , \tag{3.79}$$

which can be rearranged to read

$$G_{ns}^{ij} = \int_0^\infty dr\ r^{n-\nu+2}\ e^{-ar}\ (1-e^{-\gamma r})^{J_s}\ [(a_1 g_1+g_2) + g_2\ (a_2/r + a_3/r^2)]\quad U_s(\ell,pr) \tag{3.80}$$

For the case s=2, in which U_s is the irregular Coulomb function, this integral is computed numerically. While for "s-1", we can express the G integral as a combination of the T type integral defined in Eq. (3.69).

$$G_{ns}^{ij} = (a_1 g_1+g_2)\ T_s(n+2-\nu,a,J_s,\gamma,\ell,p) + g_2\ \{a_2\ T_s (n-\nu+1,a,J_s,\gamma;\ell,p) + a_3\ T_s\ (n-\nu,a,J_s,\gamma;\ell,p)\} \tag{3.81}$$

in which a_i (i = 1, 3) and g_j (j = 1, 2) are given by Eq. (3.78) and (3.74)-(3.76).

(iii) X Integral

This last type of bound-free integrals occurs in both direct and exchange elements. X is defined by

$$X_{ns}^{ij}\ (n,a,m,b;\lambda;\nu,\gamma,J_s,\ell,p,m',b') = \int_0^\infty dr\ r^2\ (r^n\ e^{-ar})\ f_s\ (\nu,J_s,\gamma;\ell,pr)\ V_\lambda^{mm'}(m,b;m',b';r) \tag{3.82}$$

Combining (3.61), (3.66), and (3.82), X can be expressed as

$$X_{ns}^{ij} = \frac{(m+m'+\lambda+2)!}{(b+b')^{m+m'+\lambda+3}} \int_0^\infty dr\ r^2\ (r^n\ e^{-ar})\ r^{-\nu}\ (1-e^{-\gamma r})^{J_s}\ U_s(\ell,pr)\ r^{-\lambda-1}\ [1-e^{-(b+b')r} \sum_{k=0}^{m+m'+\lambda+1} h(m,m';\lambda;k; b,b')\ r^k] . \tag{3.83}$$

We conveniently denote the multiplicative factor by "X_o".

$$X_o = \frac{(m+m'+\lambda+2)!}{(b+b')^{m+m'+\lambda+3}} ,$$

and rewrite the integral as

$$X^{ij}_{ns} = X_o \int_0^\infty dr\, r^{n+l-\nu-\lambda}\, e^{-ar}\, (1-e^{-\gamma r})^{J_s}\, U_s(\ell,pr)\, U_s(\ell,pr)$$
$$[1-e^{-(b+b')r} \sum_{k=0}^{m+m'+\lambda+l} h(m,m';\lambda,k;b,b')\, r^k] \quad . \tag{3.84}$$

For the case "s=2", in which U_s is the irregular Coulomb function, we perform a numerical computation of the integral; while, for "s=1", we express X as a combination of T type integrals

$$X^{ij}_{ns} = X_o \{T_s(n+l-\nu-\lambda,a,J_s,\gamma;\ell,p) - \sum_{k=0}^{m+m'+\lambda+l} h(m,m';\lambda,k;b,b')$$
$$T_s\,(n+k+l-\nu-\lambda,a,b+b',J_s,\gamma;\ell,p)\} \tag{3.85}$$

which enables us to evaluate the integrals analytically.

3. Free-Free Type Integrals

These integrals are evaluated numerically except possibly in a few cases.

(i) A Integrals

$$A^{ij}_{st}(\ell_1,j_s,\gamma_1,\ell',q;\ell_2,j_t,\gamma_2,\ell,p;Z) = \int_0^\infty dr\, r^2\, [r^{-\ell_1}(1-e^{-\gamma_1 r})^{j_s}$$
$$U_s(\ell',gr)]\quad [T_\ell - 2(Z-1)/r - p^2]\, [r^{-\ell_2}\,(1-e^{-\gamma_2 r})^{j_t}$$
$$U_t(\ell,pr)] \tag{3.86}$$

in which we have used the expressions (3.66) of the free functions f_s and f_t. In the special case: "$\ell_2=1$, $j_t=0$", the integral vanishes identically since U_t/r satisfies the Coulomb differential equation. Otherwise, we have to calculate expressions of the type:

$$W(r) = [T_\ell - \frac{2(Z-1)}{r} - p^2]\ [r^{-\ell_2}\ (1-e^{-\gamma_2 r})^{j_t}\ U_t(\ell,pr)]. \tag{3.87}$$

To start with, we have

$$-\frac{1}{r^2}\frac{d}{dr}\ (r^2\ \frac{d}{dr})\ [r^{-\ell_2}\ (1-e^{-\gamma_2 r})^{j_t}\ U_t(\ell,pr)] = r^{-\ell_2}$$

$$(1-e^{-\gamma_2 r})^{j_t}\ \frac{d^2}{dr^2}\ U_t(\ell,pr) + 2r^{-\ell_2-1}\ (1-e^{-\gamma_2 r})^{j_t-1}$$

$$\{(\ell_2-1)\ (1-e^{-\gamma_2 r}) - j_t\gamma_2 r\ e^{-\gamma_2 r}\ \frac{d}{dr}\ U_t(\ell,pr) - r^{-\ell_2-2}$$

$$(1-e^{-\gamma_2 r})^{j_t-2}\ \{(\ell_2 - 1)\ (1 - e^{-\gamma_2 r})\ [\ell_2(1-e^{-\gamma_2 r})$$

$$- 2j_t\gamma_2 r\ e^{-\gamma_2 r}] - j_t\ \gamma_2^2\ r^2\ e^{-\gamma_2 r}\ (1-j_t\ e^{-\gamma_2 r})\ U_t(\ell,pr)\ ; \tag{3.88}$$

then using the Coulomb differential operator, we have

$$-r^{-\ell_2}\ (1-e^{-\gamma_2 r})^{j_t}\ [\frac{d^2}{dr^2} + \frac{2(Z-1)}{r} - \frac{\ell(\ell+1)}{r^2} + p^2]\ U_t\ (\ell,pr) = 0. \tag{3.89}$$

Combining Eqs. (3.87) through (3.89), W(r) reduces to

$$W(r) = 2r^{-\ell_2-1} (1-e^{-\gamma_2 r})^{j_t-1} \{(\ell_2-1)(1-e^{-\gamma_2 r}) - j_t\gamma_2 r\, e^{-\gamma_2 r}\}$$

$$\frac{d}{dr} U_t(\ell,pr)\, -r^{-\ell_2-2} (1-e^{-\gamma_2 r})^{j_t-2} \{(\ell_2-1)(1-e^{-\gamma_2 r})$$

$$[\ell_2(1-e^{-\gamma_2 r}) - 2\, j_t\gamma_2\, r\, e^{-\gamma_2 r}] - j_t\, \gamma_2^2\, r^2\, e^{-\gamma_2 r}$$

$$(1-j_t\, e^{-\gamma_2 r})\}\ \ U_t(\ell,pr)\ .$$

The integral can now be written explicitly as

$$A^{ij}_{st} = \int_0^\infty dr\, r^{-\ell_1-\ell_2} (1-e^{-\gamma_1 r})^{j_s} (1-e^{-\gamma_2 r})^{j_t-2} U_s(\ell',qr)$$

$$[W_1(r)\, \frac{d}{dr} U_t\ (\ell,pr) + W_2(r)\, U_t\ (\ell,pr)] \qquad (3.90)$$

in which

$$W_1(r) = 2r\ (1-e^{-\gamma_2 r})\ [(\ell_2-1)\ (1-e^{-\gamma_2 r}) - j_t\gamma_2 r\, e^{-\gamma_2 r}]\ ,$$

and

$$W_2(r) = (1-\ell_2)\ (1-e^{-\gamma_2 r})\ [\ell_2(1-e^{-\gamma_2 r}) - 2\, j_t\gamma_2\, r\, e^{-\gamma_2 r}]$$

$$+ j_t\, \gamma_2^2\, r^2\, e^{-\gamma_2 r}\ (1-j_t\, e^{-\gamma_2 r})\ .$$

This integral is evaluated numerically for all combinations of s(=1,2) and t(=1,2).

(ii) I Integrals

This free-free type integral is defined by

$$I^{ij}_{s_t}(n,a,\ell_1,j_s,\gamma_1,\ell',q\ ;\lambda;n',a',\ell_2,j_t,\gamma_2,\ell,p) = \int_0^\infty dr\, r^2$$

$$f_s(\ell_1,j_s,\gamma_1;\ell',qr) = U^{\lambda}_{nn'}(n,a;n',a';r)\ f_t(\ell_2,j_t,\gamma_2;\ell,pr)$$

(3.91)

in which we define the modified potential function by

$$U^{\lambda}_{nn'}(r) = V^{nn'}_{\lambda}(r) - \frac{\alpha_{nn'}}{r^{\lambda+1}}\delta_{\lambda o} \quad . \tag{3.92}$$

We recall here that for large $r(r \geq R_o$, where R_o is large), the potential function $V^{nn'}_{\lambda}$ behaves as $\alpha_{nn'}\, r^{-(\lambda+1)}$, then $U^{\lambda}_{nn'}$ behaves as

$$U^{\lambda}_{nn'}(r) \underset{r\to\infty}{\longrightarrow} (1-\delta_{\lambda o})\frac{\alpha_{nn'}}{r^{\lambda+1}} + \text{Exponentially decreasing} \tag{3.93}$$

terms in which the long range term vanishes for "$\lambda=0$" transitions.

Hence, in order to evaluate this integral, we conveniently divide the integration domain in the following manner

$$I^{ij}_{st} = \int_0^{R_o} dr\, r^{2-\ell_1-\ell_2}\,(1-e^{-\gamma_1 r})^{j_t}\, U_s(\ell',qr)\, U^{\lambda}_{nn'}(r)\, U_t(\ell,pr)$$

$$+ \int_{R_o}^{\infty} dr\, r^{2-\ell_1-\ell_2}\,(1-e^{-\gamma_1 r})^{j_s}\,(1-e^{-\gamma_2 r})^{j_s}\, U_s(\ell',qr)\,\frac{\alpha_{nn'}}{r^{\lambda+1}}$$

$$(1-\delta_{\lambda o})\, U_t(\ell,pr). \tag{3.94}$$

in which the functions f_s and f_t are replaced by the expressions given in Eq. (3.66). The first integral can be evaluated numerically since the integrand dies off exponentially for large r as indicated in Eq. (3.93). The second integral vanishes for transitions with "$\lambda=0$". Otherwise, we choose R_o large enough for the regularizing factors to converge to unity and for the Coulomb functions to be replaced by their asymptotic expansions (Appendix D).

The integral then reads

$$\alpha_{nn'} \int_{R_o}^{\infty} dr\, r^{2-\ell_1-\ell_2}\, U_s^A(\ell',qr)\, r^{-\lambda-1}\, U_t^A(\ell,pr) \ .$$

Now, we conveniently introduce the parameter

$$L = \lambda + \ell_1 + \ell_2 - 2 \qquad (= 1, 2, 3, \ldots) \ ,$$

and define a new of integrals

$$J_{st}\ (\ell',g;L;\ell,p) = \int_{r_o}^{\infty} dr\, r^{-(L+1)}\, U_S^A(\ell',qr)\, U_t^A(\ell,pr) \ . \tag{3.95}$$

which can be evaluated analytically (Appendix E) by expanding the Coulomb functions in the asymptotic regions (keeping terms up to the order of r^{-3} only) and expressing the integral as a linear combination of a simpler type of integrals

$$K_{st}\ (\ell',q;n;\ell,p) = \int_{R_o}^{\infty} dr\, r^{-(n+1)}\, C_s(\ell',qr)\, C_t(\ell',pr)$$
$$(n = 1, 2, 3, \ldots) \tag{3.96}$$

in which

$$C_1(\ell,kr) = \sin\theta_\ell(kr)$$
$$C_2(\ell,kr) = \cos\theta_\ell(kr)$$

where $\theta_\ell(kr) = kr + \frac{(Z-1)}{k}\ \ell n\ 2\ kr - \ell\ \pi/2 + \sigma_L$, σ_L being the Coulomb phase.

Then using proper trigonometric relations (Appendix E), the K integral may be reduced to a combination of the exponential type integrals

$$\Gamma(n;a,b) = \int_{R_o}^{\infty} dr\, r^{-(n+1+ib)}\, e^{iar} \qquad (n = 1, 2, \ldots) \tag{3.97}$$

which are integrated by parts until convergence is achieved.

(iii) ε Integrals

$$\varepsilon_{st}^{ij}(\ell_1,j_1,\gamma_1,\ell',q,n,a;\ell_2,j_2,\gamma_2,\ell,p,n',a';Z,E) = \int_0^{\infty} dr\, r^2 \left(r^{n'} e^{-a'r}\right) f_s(\ell_1,j_s,\gamma_1;\ell',qr) \int_0^{\infty} dr\, r^2 f_t(\ell_2,j_t,\gamma_2;\ell,pr) \left[T_\ell - 2\,Z/r - E\right] \left(r^{n} e^{-ar}\right) + \int_0^{\infty} dr\, r^2 \left(r^{n} e^{-ar}\right) f_t(\ell_s,j_t,\gamma_2;\ell,pr) \int_0^{\infty} dr\, r^2 f_s(\ell_1,j_s,\gamma_1;\ell',qr) \left[T_{\ell'} - 2\,Z/r\right] \left(r^{n'} e^{-a'r}\right) \tag{3.98}$$

in which the integrals of the bound-free types T and B.

In order to simplify notations, we use Eqs. (3.66) and rewrite Eq. (3.98) as

$$\varepsilon_{st}^{ij} = t_1\, B_1 + t_2\, B_2 \tag{3.99}$$

in which

$$t_1 = \int_0^{\infty} dr\, r^{n'+2-\ell_1}\, e^{-a'r}\, (1-e^{-\gamma_1 r})^{j_s}\, U_s(\ell',qr) \quad ,$$

$$t_2 = \int_0^{\infty} dr\, r^{n+2-\ell_2}\, e^{-ar}\, (1-e^{-\gamma_2 r})^{j_t}\, U_t(\ell,pr) \quad ,$$

$$B_1 = \int_0^{\infty} dr\, r^{2-\ell_2}\, (1-e^{-\gamma_2 r})^{j_t}\, U_t(\ell,pr)\, \left[T_\ell - 2\,A/r - E\right] \left(r^{n} r^{-ar}\right) \quad ,$$

and

$$B_2 = \int_0^\infty dr\ r^{2-\ell_1}\ (1-e^{-\gamma_1 r})^{j_s}\ U_s(\ell',qr)\ [T_{\ell'} - 2\ Z/r]\ (r^{n'}e^{-a'r})$$

The integrals t_1 and t_2 are T type integrals defined in Eq. (3.3.17):

$$t_1 = T_s(n'+2-\ell_1, a', j_s, \gamma_1, \ell', q)$$

and

$$t_2 = T_t(n+2-\ell_2, a, j_t, \gamma_2, \ell, p)\ .$$

Then using expressions of the type (3.72), B_1 reduces to

$$B_1 = \int_0^\infty dr\ r^{2-\ell_2+n}\ (1-e^{-\gamma_2 r})^{j_t}\ e^{-ar}\ [a_1+a_2/r]\ U_t(\ell,pr) \qquad (3.100)$$

in which

$$a_1 = -(a^2 + E)\ ,$$

$$a_2 = 2[(n+1)\ a-Z]\ ,$$

and $$a_3 = \ell(\ell + 1) - n(n + 1)$$

This integral is evaluated numerically for "s=0"; while, for "s=1", it can be expressed as a linear combination of T-type integrals:

$$B_1 = a_1\ T_t(n+2-\ell_3, a, j_t, \gamma_2, \ell, p) + a_2\ T_t(n+1-\ell_2, a, j_t, \gamma_2, \ell, p) + a_3\ T_t(n - \ell_2, a, j_t, \gamma_2, \ell, p) \qquad (3.101)$$

Similarly, B_2 reduces to

$$B_2 = \int_0^\infty dr\ r^{2+n'-\ell_2}\ e^{-a'r}\ (1-e^{-\gamma_1 r})^{j_s}\ [a_1' + a_2'/r + a_2'/r^2]\ U_s(\ell',qr) \qquad (3.102)$$

in which

$$a_2' = -a'^2 \quad ,$$

$$a_2'' = 2[(n'+1)\ a' - z] \quad ,$$

and

$$a_3' = \ell'(\ell' + 1) - n'(n' + 1) \quad .$$

Again, this integral is evaluated numerically for "s=2", while for "s=1", it can be expressed as a linear combination of T-type integrals:

$$B_2 = a_1' T_s(n'+2-\ell_1, a', j_s, \gamma_1, \ell', q) + a_2' T_s(n'+1-\ell_1, a', j_s, \gamma_1, \ell', q) + a_2' T_s(n' - \ell_1, a', j_s, \gamma_1, \ell', q) \quad . \tag{3.103}$$

(iv) H Integral

This last type of free-free integral is given by

$$H_{st}^{ij}(n,a,\ell_1,j_1,\gamma_i,\ell',q;\lambda;n',a',\ell_2,j_2,\gamma_2,\ell,p) = \int_0^\infty dr\ r^2 \left[r^{-\ell_1} (1-e^{-\gamma_1 r})^{j_s} U_s(\ell',qr)\right] (r^{n'} e^{-a'r}) \int_0^\infty dx\ x^2 \left[x^{-\ell_2} (1-e^{-\gamma_2 x})^{j_t} U_t(\ell,px)\right] (x^n e^{-ax}) \frac{x_<^\lambda}{x_>^{\lambda+1}} \tag{3.104}$$

in which $x_< = \min(x,r)$, and $x_> = \max(x,r)$.

In order to evaluate this integral, we break the integration domain (over x) into 2 intervals: [0,r] U[r,∞). Eq. (3.104) now reads

$$H_{st}^{ij} = \int_0^\infty dr\ r^{n'+2-\ell_1} e^{-a'r} (1-e^{-\gamma_1 r})^{j_s} U_s(\ell',qr) \left[r^{-\lambda-1} \int_0^\infty dx\ x^{n+\lambda+2-\ell_2} e^{-ax} (1-e^{-\gamma_2 x})^{j_t} U_t(\ell,px) + r^\lambda \int_r^\infty dx\ x^{n+1-\lambda-\ell_2} e^{-ax} (1-e^{-\gamma_2 x})^{j_t} U_t(\ell,px)\right] \quad . \tag{3.105}$$

We then rewrite the integral whose domain is $[r,\infty]$ as the difference of two integrals whose domains are $[0,\infty]$ and $[0,r]$, respectively. Hence:

$$H^{ij}_{st} = \int_0^\infty dr\, r^{n'+2-\ell_1} e^{-a'r} (1-e^{-\gamma_1 r})^{j_s} U_s(\ell,qr) \{r^{-\lambda-1} \int_0^r dx\, x^{n+\lambda+2-\ell_2} e^{-ax} (1-e^{-\gamma_2 x})^{j_t} U_t(\ell,px) - r^2 \int_0^r dx\, x^{n+1-\lambda-\ell_2} e^{-ax} (1-e^{-\gamma_2 x})^{j_t} U_t(\ell,px) + r^\lambda \int_0^\infty dx\, x^{n+1-\lambda-\ell_2} e^{-ax} (1-e^{-\gamma_2 x})^{j_t} U_t(\ell,px)\}. \quad (3.106)$$

We now introduce the "Inner" integrals defined by

$$T_t(n,a,j,b,\ell,p;r) = \int_0^r dx\, x^n e^{-ax} (1-e^{-bx})^j U_t(\ell,px) \quad (3.107)$$

and rewrite Eq. (3.106) as

$$H^{ij}_{s_t}(\lambda) = \{\int_0^\infty dr\, r^{n'+2+\lambda-\ell_1} e^{-a'r} (1-e^{-\gamma_1 r})^{j_s} U_s(\ell',qr) \int_0^\infty dr\, r^{n+1-\lambda-\ell_2} e^{-ar} (1-e^{-\gamma_2 r})^{j_t} U_t(\ell,pr)\} + \int_0^\infty dr\, r^{n'+2-\ell_1} e^{-a'r} (1-e^{-\gamma_1 r})^{j_s} U_s(\ell',qr) [r^{-\lambda-1} T_t(n+\lambda+2-\ell_2,a,j_t,\ell,p;r) - r^\lambda T_t(n+1-\lambda-\ell_2,a,j_t,\gamma_2, \ell,p;r)] \quad (3.108)$$

The term in { } is a product of 2 T type integrals defined in Eq. (3.69). The second term involves two "inner" integrals and is thus evaluated numerically for

all combinations of s and t.

In conclusion, we remark that most of the computation time is spent in the numerical evaluation of free-free type integrals discussed above. Reduction in computation time is probable if adequate analytic solutions can be found for these integrals as well as for bound-free type integrals which involve an irregular Coulomb function. We found out that this task is not an easy one to accomplish. Other limitations on the evaluation of these specific integrals are associated with the numeric Coulomb function generator, RCWFN.[40] The irregular Coulomb function should Be evaluated accurately enough at small r to get a good result for the bound-free integrals. However, for $\ell=0$, both the regular and irregular functions, as well as their first deviatives which are furnished by RCWFN are cut off at small ρ. This results in a reduction in the degree of accuracy desired for these integrals. It is worth noting here that the calculated cross sections; the $1s \rightarrow 2s$, for example; can be as small as 10^{-8} while the Coulomb functions, or their first derivatives are only accurate to 6 or at most 7 significant figures for small ρ. Despite this, we did not choose to avoid these problems by approximating the irregular Coulomb function as a linear combination of 2 regular functions[8,9]; instead, we have chosen to optimize the integration scheme so as to use the least number of

mesh points and the largest mesh size possible, without sacrificing the accuracy of the results. The eleven-point Newton-Cote type formula used will be introduced in Appendix F.

CHAPTER IV

APPLICATIONS AND RESULTS

In this chapter the collision strengths and excitation rates for C^{5+} and O^{7+} obtained in our calculation, are described and compared with results from other theoretical methods. We present in Section A the optimized short range bases used in the expansions of the trial scattering wave functions. In Section B we discuss the results obtained for excitation cross sections, and show the results for elastic cross sections as well, when the 3s-3p close coupling set is used. Section C presents the results obtained above the ionization energy using the same basis, but in terms of the conventional collision strengths (Ω). Positions and widths of resonances under the n=3 hydrogenic level in C^{5+} and O^{7+} are presented in Section D; comparison is made with results from the complex rotation method. Finally, resonance enhancement of excitation rates is discussed in Section E where thermally averaged cross sections for the 2s and 2p excitation of C^{5+} and O^{7+} are presented and compared with theory

A. Short Range Basis

The trial wave function defined in Eq. (2.14) contains a short range part which has been expanded

in a set of Slater orbitals of the type $r^{\ell}e^{-\zeta_j r}$ in which ℓ is the orbital angular momentum and $\{\zeta_j\}$ is a set of exponents, properly chosen to get optimum results in different energy intervals.

The basis set associated with the 3s-3p set had to be scaled with energy. As the incident electron energy increases, larger exponents are needed in order to represent the rapid oscillations in the wavefunction. These exponents are listed in Tables III and IV, columns (a). We had to use 3 different sets for C^{5+}. The numbers in the first column of Table III form a decreasing geometric progression of common ratio 1.3 and a maximum value of 15. The next 2 columns show the same progression with the lowest term(s) deleted and replaced by one (or more) term(s) larger than 15, whose scaling ratio is 1.2. Furthermore, Table IV shows four different sets for O^{7+}, which have been constructed and optimized in a similar manner. We note here that the exponents also scale in some manner with the nuclear charge. This is clear whenever the numbers in Tables III and IV are compared. This scaling with Z is not accidental, we actually tested that matter by varying the highest exponent keeping the same common ratio, or varying the common ratio itself, until we had the right choice of bases that would guarantee stability and accuracy of the results

for a particular target in different energy intervals.

The type of exponents described above was not adequate in the resonance region, between the n=2 and n=3 excitation thresholds. An extended basis is needed there in order to represent the wave functions. The sets used are listed in Tables III and IV, columns (b). The first five elements in each set form a decreasing geometric progression of a common ratio 1.3; then a decreasing ratio from 1.40 down to 1.85 is used for the remaining elements.

The size of each basis has also been optimized. Fifteen Slater orbitals have proved to be sufficient for our purposes. Adding more elements in the basis produced no significant change in the calculated cross sections, however it would have increased the computation time. On the other hand, using fewer elements resulted in a lack of accuracy.

B. Excitation Cross Sections

In this section, we discuss the results obtained using the 3s-3p basis in the energy range from just above the n=2 excitation threshold to around 5 times that threshold.

We found that, at a particular energy in the region specified above, the results of the variational pseudo-state calculations agreed with the results of the

Coulomb Born with exchange approximation (CBX) for some total angular momentum (L_{MAX}). Then above L_{MAX}, the CBX partial cross sections were used. L_{MAX} decreased from L=5 near the n=2 threshold to L=2 near 5 times that threshold in C^{5+}, and to L=0 in O^{7+}. It has been observed that excitation cross for O^{7+} converged more rapidly to those obtained using the simple CBX approximation, than those for C^{5+}. This has been expected since CBX becomes more reliable as the nuclear charge increases. Having determined these facts, it seemed logical that only CBX results be used at higher energies ($x \gtrsim 5$).

The spin weighted partial cross sections for the 2s and 2p excitations of C^{5+} and O^{7+} are given in Tables V-VIII. These tables contain basically the 3s-3p results except for high L contributions (σ_{high}) which were determined using CBX. The values of singlet L=0 which appear with a * have been corrected for pseudo-resonances. Table IX shows the energy region in which the K matrices were fitted as discussed earlier (see Section III.E), the pseudopoles were extracted, and the cross sections were recalculated. This is the only partial wave that showed appreciable pseudo-resonance behavior at energies above ionization (x = 1.33). However, another spurious K matrix pole occurs around x = 1.17 in the region below the first

pseudothreshold at x = 1.305. This pseudoresonance has a significant effect on the singlet S, P and F as well as the triplet P and F partial excitation cross sections for C^{5+} and O^{7+}. We had decided to use a larger close coupling set in that crucial energy region (as will be discussed in the next sections), hence we did not average over this pseudoresonance. Further analysis of Tables V through VIII shows, beyond any doubt, what has been observed in previous calculations.[7,9] Specifically, the 2s excitation is dominated by low partial waves even at relatively high energies. The high L contribution (σ_{high}) amounts to no more than 35 percent of the total cross section at x = 4.9 in C^{5+} and 32% at x = 4.69 in O^{7+}. In contrast, 2p excitation is dominated by high partial waves even at relatively low energies. The high contribution in this case increases rapidly from 2% at ionization to 94% at x~5 in both C^{5+} and O^{7+}. This behavior results from the fact that the effective transition potential is long ranged for the optically allowed 1s→2p transition; short ranged for 1s→2s. As will be discussed in the next section, it is the 2s excitation cross section which is sensitive to the choice of close coupling bases.

Finally, Tables X and XI show the elastic (1s→1s) partial cross sections for C^{5+} and O^{7+}

simultaneously. The cross sections are given in units of $10^{-3}\ \pi a_o^2$. No corrections have been made for pseudo-resonances. High L contributions have not been calculated either. The 1s→1s cross sections are clearly dominated by low partial waves. Our main interest has been in excitations of the C^{5+} and O^{7+} ions, hence no further investigation of the elastic cross section has been made.

C. The Convenient Ω

In this section we present our results in the energy region above ionization ($x \gtrsim 1.33$) in terms of the dimensionless collision strength (the convenient Ω) which is given for hydrogenic ions by

$$\Omega_{i\to j} = 2k_i^2\ \sigma_{i\to j} \tag{4.1}$$

where $\sigma_{i\to j}$ is the corresponding excitation cross section (in units of πa_o^2). Table XII shows our results for the calculated collision strengths for the 2s and 2p excitations of C^{5+} and O^{7+} as a function of the dimensionless scaled energy, x.

For convenience of people interested in using this data, we have fitted the collision strengths by the semi-empirical analytic formula for spin allowed

transitions

$$\Omega(x) = a \ln x + b + c/x + d/x^2 \qquad (4.2)$$

with a = 0 for the 2s excitation. In fact, the collision strength for optically allowed long ranged dipole transitions (like the 1s-2p), behaves logarithmically for large x, while it approaches an asymptotic value as $x \to \infty$ for optically forbidden transitions (like the 1s-2s). The coefficients (COEF) are given in Table XIII. The fits for C^{5+} are accurate to better than 1% for the 2p excitation, but have a worst case error of 5% for the 2s excitation. Similarly, the fits for the 2p and 2s excitations of O^{7+} have a worst case error of 4%. The fits could not be improved by adding another term ($\sim 1/x^3$).

Many theoretical calculations are available in this energy range. Figures V-VIII show our results compared to most of these calculations. We discuss first the 2s excitation. For both ions (C^{5+} and O^{7+}), our 2s collision strengths have a different shape, as well as are smaller at low energies than in all other works. We have found a minimum in the vicinity of x = 2. This minimum also occurred in a previous calculation on He^+,[7] which utilized the same 3s-3p close coupling set. It has been observed that the

position of the minimum (x_m) shifts towards the ionization threshold as the nuclear charge increases (x_m ~ 1.93 for He^+, ~1.73 for C^{5+} and ~1.60 for O^{7+}). Further calculations on higher Z hydrogenic ions would certainly reveal the behavior of this minimum. We would like to mention here that the standard 3 state close coupling calculations by Seaton and Hayes,[15] show a shallow minimum at a lower energy not shown in Fig. V, since it lies in the resonant energy region.

Other calculations which yield dramatically different results from ours in the low energy region, particularly around the x=2, are the Coulomb Born with exchange (CBX),[16] the infinite Z hydrogenic method (IZH),[18] distorted wave (DW) with exchange by Mann,[16] and Coulomb Born without exchange (CB).[16,19] Other distorted wave calculations by Balija and McDowell[17] as well as by Peek (quoted by Ref. 13) lie rather close to IZH and are thus indistinguishable on the scale of Fig. V. In fact, since the application of DW methods to highly stripped ions have become very popular, we find it worth noting that at x=2, our results are about 29% below DW for C^{5+} and 26% for O^{7+}. This substantial difference makes the use of DW in that energy region rather questionable. Coulomb Born results are even substantially larger than ours for 2s excitations. The three points (dark triangles) shown on Fig. V were

available from a second order potential calculation.[41]

On the other hand, calculations of the 2p excitation cross sections by various methods agreed rather well at all energies. Except for CB results, they are all almost indistinguishable on the scales of Figs. VII and VIII. Although the 3CC result is about 11% higher at ionization, it is only 3% by x=2. DW results agreed with ours to a large extent for x=2. The same is true for CBX results. The IZH results for the 2p excitation of C^{5+} which are shown in Fig. VII give a clear idea of how well different methods work for excitations which involve a long ranged dipole transition potential, such as the 2p excitation. We conclude that the inclusion of pseudostates is rather important for the 2s but not the 2p excitation in highly stripped ions for the reasons discussed above.

D. Results in the Resonance Region

We report in this section our results for resonances between the n=2 and n=3 thresholds. In order to have a feeling for the nature of these resonances, we consider an electron incident on a hydrogenic ion in this energy range. Temporary bound (autoionizing) states can be formed with the excited electron of the ion. These states have the approximate configuration (3ℓ, $n\ell'$; $\ell = 0,1,2,$; $\ell' = 0,1,2,...$) and are expected to appear

as resonances in the scattering process. In fact, hydrogenic ions have an infinite series of resonances below each excitation threshold. This is due to the long range Coulomb potential. The structure obtained below the n=3 threshold is quite complex due to the degeneracy of the 2s and 2p states.

The variational method is particularly accurate when only a few excited channels are open, as is the case in this energy region. The 14 state close coupling set (6s-5p-2d-1f) has been used. Energies and parameters of this set are listed in Table I. This set has been proved[6] capable of yielding resonance energies and widths rather accurately in comparison with other theoretical methods, the complex rotation, for instance. We have restricted the total angular momentum to $L \leq 4$, and have found resonances in all partial waves (^1S through ^3G).

Positions (E_o) and widths (Γ) of these resonances can be determined by investigating the behavior of the eigenphase sum (δ_T); the sum of eigenvalues of the K matrix. In fact, δ_T changes by π past a resonance. We have then fitted the eigenphase sums to the equation

$$\delta_T(E) = \delta_B(E) + \tan^{-1}\left(\frac{\Gamma/2}{E_o - E}\right) \qquad (4.3)$$

Here δ_B is the background phase shift which is a slowly varying function of energy over a particular region. Values for positions (in terms of the scaled energy, x_{12}) and width (in Rydbergs, Γ) are given in Table XIV, where they are compared with those of HO who used the complex rotation method with a large basis of Hylleras type functions.[42] We are not aware of other numerical results for these hydrogenic ions (C^{5+}, O^{7+}). Results of Hayes and Seaton are available for C^{5+} only in graphical form.[14]

It is evident that the agreement between this pseudostate variational calculation and the complex rotation method is good in cases where results of both types are available (^1S, ^1P and ^3P). This kind of agreement is not accidental. Both methods have agreed pretty well in previous work on resonances in neutral system (H),[43] as well as in ions (He^+).[6] However, we were not able to detect the third ^1S resonance which is a very narrow one. (This is probably due to our basis being inefficient in describing the proper configuration of this resonance.)

Further investigation of Table XIV shows that almost all resonances have widths which increase slightly with Z. Besides, widths vary from very narrow (^3S and ^3F) to very broad (^1S and ^1G). The width of the ^3F resonance in C^{5+} does not exceed 0.0009 eV, while

that of the ^1G resonance in O^{7+} exceeds 0.7 eV. Finally, comparison was made with results by Callaway and Ho, who obtained many of these resonances (all but ^3S) using the complex rotation method with configuration interaction type functions (their numbers are not shown in Table XIV).[44] Our results agree to a good extent with theirs: our resonance positions are slightly higher than theirs, widths are either as broad or slightly wider.

The 2s and 2p excitation cross sections of C^{5+} and O^{7+} in this energy region are listed in full in Tables XV and XVI, for all total angular momenta (L=0-4) (energies are given in terms of the scaled parameter x). The calculations were made at values of x which are either scattered in regions away from resonances (for example, x = 1.01, 1.03, 1.05, 1.09, 1.14, 1.16) in order to represent the background cross section, or are very closely situated around resonances.

The K matrix fitting technique has been used to study the cross sections in this region. The examples shown in Figs. IX and X illustrate the ^1P and ^1F contributions to the 1s→2s cross section in C^{5+}, while those shown in Figs. XI and XII illustrate the ^1D and ^1F contributions to the 1s→2p cross section in O^{7+}. In all these four, as well as in other cases considered,

calculations were made between x = 1.01 and x = 1.16: at 41 energies for ^1P, 25 for ^1F in C^{5+}; at 25 energies for ^1D, 19 for ^1F in O^{7+}. The K matrix fit was used to obtain results for 1851 energies (on a grid with $\Delta x = 0.0001$). This calculation will be helpful in determining the contribution of the resonance region to thermal average cross sections (as will be discussed in the next section).

The total excitation cross sections in the resonance region are shown in Figs. XIII-XVI. The resonances fall into 2 groups, separated by about 1 Ry in C^{5+} and 2 Ry in O^{7+}. The resonances in the lower group can be described as those in which both electrons occupy the same shell (n = n'=3). The upper group represents the case in which the 2 electrons occupy the levels n=3 and n=4. As discussed above, an infinite number of these groups exist under the n=3 threshold, of which we have chosen to study the first two. Careful analysis of the graphs show undoubtedly that the resonance contribution to rate coefficients will be small.

We would like to mention here, that so far, no experimental observation of these resonances has been made in these highly stripped ions. We suggested[37] that if suitable ionic beams can be prepared, observation of these resonances may be possible, since no matter how narrow the individual resonances may be, the (3ℓ,

$3\ell'$) structure, for instance, extends over an energy range of ~9 eV in C^{5+}, 12 eV in O^{7+}, and the (3ℓ, $4\ell'$) structure extends over ~5 eV in C^{5+}, ~8 eV in O^{7+}.

E. Thermally Averaged Cross Sections

Accurate excitation rates for electron impact excitation of hydrogenic as well as other positive ions, are required in the analysis of the spectra of hot plasmas. We shall consider here the thermally averaged cross section which is proportional to the rate coefficient.

We assume a Maxwellian distribution of incident electron velocities (v)

$$P(v) = \left(\frac{m}{2\pi K\theta}\right)^{3/2} e^{-mv^2/2K\theta} \tag{4.4}$$

in which K is the Boltzmann's constant, m is the electron mass, and θ is the electron temperature. The thermally averaged cross section is then defined by

$$\bar{\sigma} = \frac{1}{v_A} \int P(v)\ v\ \sigma(v)dv \tag{4.5}$$

where $\sigma(v)$ is the excitation cross section and v_A is the average thermal velocity

$$v_A = (8K\theta/\pi m)^{1/2} \tag{4.6}$$

A proper change of variables

$$x = mv^2/2E_x \tag{4.7}$$

where E_x is the excitation energy; leads to

$$\bar{\sigma} = q^2 \int_1^\infty x\, \sigma(x) e^{-qx}\, dx \tag{4.8}$$

in which

$$q = E_x/K\theta \tag{4.9}$$

The integral may be rewritten as

$$\bar{\sigma} = \frac{q}{2K\theta} \int_1^\infty e^{-qx}\, \Omega(x) dx\ , \tag{4.10}$$

where we have used the definition of the collision strength (4.1) and Eq. (4.9)

$$\Omega(x) = 2\, xE_x\sigma(x) = 2x\, qK\theta\sigma(x) \tag{4.11}$$

the integration domain has been conveniently divided into two parts

$$\bar{\sigma} = A_r + B \tag{4.12}$$

with

$$A_r = q^2 \int_1^{x_o} x\, e^{-qx}\, \sigma(x)\, dx \tag{4.13}$$

in which $x_o = 1.1852$ (the position of the n=3 threshold), and

$$B = \frac{q}{2K\theta} \int_{x_o}^{\infty} e^{-qx}\, \Omega(x)\, dx \ . \tag{4.14}$$

The integral A_r computes the contribution of the resonance region. The cross sections used in the integrand are those obtained from the K matrix fit to the results of the 14 states set. In the fitting procedure, we re-evaluated the cross sections at intervals of $\Delta x = 0.0001$. This enabled us to perform a rather accurate numeric integration over this region (Simpson's integration rule has been sufficient to yield reliable results). In the energy region above the n=3 threshold ($x > x_o$), we have used the empirical fit to the collision strength given by Eq. (4.2). The contribution, B, from this region to the thermally averaged cross section is then given by

$$B = \frac{1}{2K\theta}\{(a\ \ell n\ x_o + b + \frac{dq}{x_o})e^{-qx_o}$$

$$+ (a + cq - dq^2)E_1(qx_o)\} \qquad (4.15)$$

in which E_1 is an exponential integral function defined by

$$E_1(qx_o) = \int_{x_o}^{\infty} \frac{e^{-qx}}{x}\,dx \qquad (4.16)$$

Our results are shown in Tables XV and XVI where the thermal average cross sections at selected temperatures T (in KeV), are listed, and in Figs. XVII and XVIII where they are compared with those obtained by fitting the results of the DW calculation by Mann.[16] The DW averages for the 2p excitation agree to better than 1% with ours above T = 1 KeV in both C^{5+} and O^{7+}, and are only a few percent higher at lower temperatures. On the contrary, the DW averages for the 2s excitations are considerably higher, by more than 20% around 400 eV in C^{5+} and by a little less than 20% around 500 eV in O^{7+}. It is worth noting here the range of temperatures is considered such that the 2s and 2p excited states of the ions do exist. The use of a non-relativistic Maxwellian velocity distribution for the incident electrons at the temperatures of interest here, is then justified.

We have determined in this work that the resonance enhancement in the energy range under the n=3 threshold, is only a few percent over the background. We calculated the ratio A_r/A_n where

$$A_n = \frac{1}{2K\theta} \int_1^{x_o} \Omega_o(x) e^{-qx}\, dx \qquad (4.17)$$

in which $\Omega_o(x)$ represents the background collision strengths as obtained using the 14 states set and fitted by Eq. (4.2). It is worth noting here that using the 3s-3p set to represent the background in this region, would have wiped out any resonance enhancement, since the 3s-3p cross sections are almost 10% larger for the 2s excitation and 5% for the 2p excitation, than those obtained by the larger basis. The ratio A_r/A_n (listed in Tables XVII and XVIII) show a resonance enhancement which is no more than 11% for the 2s excitation in C^{5+}, 9% in O^{7+}, and which does not exceed 5 to 6% for the 2p excitation in both ions.

The contribution of the resonance region relative to the non resonant one, has also been determined by calculating the ratio A_r/B (shown in Tables XVII and XVIII)--we recall here that the collision strength fit in the non resonant region is based on results from the 3s-3p basis--the ratio decreases rapidly with temperature. For the 2s average cross section, $A_r/B \sim 15\%$ at 0.5 KeV in

C^{5+} and at 1 KeV in O^{7+}; ~8% in C^{5+} and 7% in O^{7+} for the 2p average cross section at the same temperatures. It is evident that the resonance region contribution is dominant at low temperatures only. However, the overall effect of resonances is not as important as has been indicated by Hayes and Seaton.[14,15] In order to determine this effect, we compared the average cross sections as calculated above with those calculated if only the background were included, that is we compared 'A_r+B' to 'A_n+B'. It turned out that the resonance enhancement of the thermal average cross sections is quite small (<1% for $\theta \gtrsim 1$ KeV), except possibly at the lowest temperatures considered, where there is about a 6% resonance enhancement of the 2s average cross section, and about 3% for the 2p. Even if contributions from higher resonance groups (3ℓ, $n'\ell'$; $n' \gtrsim 5$) were included, we still think that the predictions of Hayes and Seaton that a 10 to 20 percent resonance enhancement of 1s→2s and 1s→2p rate coefficients exists,[14] are exaggerated.

In conclusion, we have determined that the background representation of the whole energy range ($x \gtrsim 1.0$) by the 3s-3p basis collision strengths is sufficient to evaluate excitation rates rather accurately, because the overestimate it makes in the resonance region about equals the actual resonance enhancement.

CHAPTER V

CONCLUSION

We have succeeded in this work in solving some important problems associated with pseudostate expansions in close coupling methods, namely that of the spurious pseudoresonances ("THE DRAGON'S TEETH"[37]) which occur under pseudothresholds. An adequate remedy has been given in terms of fitting the K matrix around the pseudopole(s), then recalculating the background cross sections in the absence of any pseudoresonant structure. We have also determined the significant effect of pseudostates on optically forbidden transitions which involve a short ranged transition potential. In fact, our calculations for C^{5+} and O^{7+} show a significant reduction (~20%) in the 2s excitation and thermal average cross sections, in comparison with the frequently used distorted wave method. However, the reduction is negligible for the optically allowed 2p excitation, where most approximation methods are as efficient as ours.

Many resonances have been detected in the energy range between the n=2 and n=3 hydrogenic levels in both ions. The resonance widths vary from the extremely narrow ^3S and ^3F ($\lesssim$ 0.001 eV) to the broad ^1S and ^1G resonances ($\lesssim$ 1 eV). However, the net effect of the two groups of resonances obtained (roughly described as the $(3\ell, 3\ell')$ and $(3\ell, 4\ell')$) is to enhance the excitation rates by no

more than a few percent; ~ 6% for the 2s and ~4% for the 2p. We believe from this evidence, that the inclusion of higher resonance series would not cause any further significant enhancement of the rate coefficients. This justifies the use of the semi-empirical representation of the collision strengths (based on results obtained using the small 3s-3p close coupling set) in order to evaluate excitation rates for hydrogenic ions.

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TABLE I

Pseudostate Parameters and Energies. Energies are in Rydbergs

j	m(j)	ζ(j)/Z	E/Z^2	m(j)	ζ(j)/Z	E/Z^2
1	0	1.0	-1.0	1	1.0	-0.25
2	0	0.5	-0.25	1	0.8	-0.02145
3	1	0.5	0.31115	1	0.5	+1.12556

	ℓ=0			ℓ=1			ℓ=2			ℓ=3	
j	m	ζ/Z	E/Z^2	m	ζ/Z	E/Z^2	m	ζ/Z	E/Z^2	m	ζ/Z	E/Z^2
1	0	1.0	-1.0	1	1.0	-0.25	2	0.5	-0.11111	3	0.5	0.0
2	0	0.5	-0.25	1	0.5	-0.11111	2	1/3	+0.00065			
3	1	0.5	-0.11111	1	1/3	-0.06219						
4	0	1/3	-0.05375	2	1/2	+0.02744						
5	1	1/3	+0.11705	1	0.2	0.90192						
6	2	1/3	+1.69818									

TABLE II

1s→2s Spin Weighted Partial Excitation Cross Sections For O^{7+} at x = 1.33 (Units 10^{-4} πa_o^2)

L	S	Kohn	In. Kohn	OAF	OMN	IOMN	B.E.
0	0	0.142	0.142	0.142	0.142	0.141	0.142(1)
	1	0.0082	0.0090*	0.0082	0.0082	0.0322*	0.0082(0)
1	0	0.352	0.353	0.352	0.352	0.353	0.352(1)
	1	0.0973	0.0975	0.0973	0.0973	0.0990*	0.0974(1)
2	0	0.0076	0.0076	0.0077	0.0077	0.0076	0.0076(1)
	1	0.129	0.129	0.129	0.129	0.129	0.129(0)
3	0	0.0020	0.0015	0.0018	0.0026*	0.0015	0.0017(3)
	1	0.0107	0.0131*	0.0109	0.0101*	0.0108	0.0108(1)
4	0	0.00085*	0.00098	0.00103	0.00093	0.00099	0.00099(6)
	1	0.00061*	0.00040	0.00039	0.00050	0.00040	0.00045(6)
5	0	0.00029	0.00023	0.00098*	0.00027	0.00023	0.00026(3)
	1	0.00023	0.00021	0.0169*	0.00024	0.00026	0.00024(3)

Table II. Starred values are regarded as anomalous and are not considered in the averaging procedure used to obtain the best estimate (B.E.). The numbers in parenthesis in the last column estimate the uncertainty in the cross sections.

TABLE III

Exponents of the Short Range Basis for Electron Scattering by C^{5+} in Different Energy Intervals

(a)			(b)
$1.0<x\leq3.0$	$3.0<x<4.0$	$4.0\leq x<5.0$	$1.0<x\leq1.1851$
15.00	18.00	25.92	15.00
11.538	15.00	21.60	11.538
8.876	11.538	18.00	8.876
6.827	8.876	15.00	6.827
5.252	6.827	11.538	5.252
4.040	5.252	8.876	3.751
3.108	4.040	6.827	2.587
2.390	3.108	5.252	1.725
1.839	2.390	4.040	1.113
1.414	1.839	3.108	0.695
1.088	1.414	2.390	0.422
0.837	1.088	1.839	0.248
0.644	0.837	1.414	0.142
0.495	0.644	1.088	0.0787
0.381	0.495	0.837	0.0426

Table III. (a) Associated with the 3s-3p close coupling set; (b) associated with the 6s-5p-2d-1f set.

TABLE IV

Exponents of the Short Range Basis for Electron Scattering by O^{7+} in Different Energy Intervals

(a)				(b)
$1.0<x\leq2.0$	$2.0<x\leq3.0$	$3.0<x<4.0$	$4.0\leq x<5.0$	$1.0<x\leq1.1851$
15.60	18.72	22.464	26.957	15.60
12.00	15.60	18.72	22.464	12.00
9.231	12.00	15.6	18.72	9.231
7.101	9.231	12.00	15.6	7.101
5.462	7.101	9.231	12.00	5.462
4.202	5.462	7.101	9.231	3.901
3.232	4.202	5.462	7.101	2.691
2.486	3.232	4.202	5.462	1.794
1.912	2.486	3.232	4.202	1.157
1.471	1.912	2.486	3.232	0.723
1.132	1.471	1.912	2.486	0.438
0.870	1.132	1.471	1.912	0.258
0.670	0.870	1.132	1.471	0.147
0.515	0.670	0.870	1.132	0.0819
0.396	0.515	0.670	0.870	0.0443

Table IV. (a) Associated with the 3s-3p close coupling set; (b) associated with the 6s-5p-2d-1f set.

TABLE V

Spin Weighted Partial and Total 1s-2s Cross-Sections for Excitation of C^{5+} (units $10^{-4}\ \pi a_o^2$)

	SINGLET						TRIPLET							
x	L=0	L=1	L=2	L=3	L=4	L=5	L=0	L=1	L=2	L=3	L=4	L=5	$^{+}\sigma_{high}$	Total σ
1.01	0.878	1.253	0.170	0.0377	0.0024	0.00026	0.0083	0.356	0.359	0.0015	0.0029	0.00058	0.000002	3.070
1.07	0.757	1.232	0.0600	0.0410	0.0028	0.00027	0.0155	0.385	0.390	0.0020	0.0023	0.00070	0.00003	2.889
1.17	0.656	0.444	0.0205	0.0485	0.0044	0.00047	0.0240	0.111	0.407	0.0112	0.0018	0.00066	0.00017	1.730
1.20	0.587	1.647	0.0133	0.181	0.0051	0.00057	0.0250	0.282	0.409	0.0153	0.0019	0.00082	0.00024	3.168
1.33	0.502*	1.016	0.0112	0.0122	0.0054	0.0011	0.0265	0.368	0.419	0.0298	0.0013	0.0012	0.00067	2.394*
1.50	0.393*	0.835	0.0230	0.0044	0.0035		0.0324	0.330	0.401	0.0600	0.0027		0.0053	2.090*
2.00	0.229	0.536	0.0728	0.0018	0.0011		0.0400	0.222	0.314	0.0918	0.0106		0.0120	1.531
2.47	0.148	0.418	0.0847	0.0070			0.0434	0.203	0.271	0.0990			0.0646	1.339
3.33	0.0870	0.227	0.0955	0.0160			0.0418	0.144	0.195	0.104			0.0937	1.004
4.00	0.0724	0.159	0.0877	0.0252			0.0450	0.133	0.167	0.107			0.110	0.906
4.90	0.0491	0.103	0.0803				0.0421	0.109	0.140				0.275	0.798

Table V. $^{+}\sigma_{high}$ is obtained using CBX. * = corrected for pseudoresonances.

TABLE VI

Spin Weighted Partial and Total 1s-2p Cross-Sections for Excitation of C^{5+} (units 10^{-4} πa_o^2)

	SINGLET						TRIPLET							
x	L=0	L=1	L=2	L=3	L=4	L=5	L=0	L=1	L=2	L=3	L=4	L=5	$^{+}\sigma_{high}$	Total σ
1.01	0.786	1.414	6.653	1.680	0.165	0.0090	0.0440	0.246	0.193	1.432	0.331	0.0250	0.0019	12.98
1.07	0.726	1.194	5.723	1.835	0.270	0.0302	0.0590	0.132	0.222	1.507	0.525	0.0784	0.0126	12.31
1.17	0.948	0.359	6.409	1.804	0.433	0.0800	0.0768	0.0560	0.267	1.561	0.796	0.198	0.0629	13.05
1.20	0.748	1.609	5.246	1.099	0.480	0.0966	0.0820	0.772	0.276	1.702	0.863	0.240	0.0876	13.30
1.33	0.534*	0.788	3.769	1.937	0.632	0.176	0.0909	0.130	0.320	1.584	1.101	0.427	0.246	11.73*
1.50	0.420*	0.608	2.757	1.883	0.760		0.107	0.108	0.349	1.511	1.302		1.510	11.31*
2.00	0.267	0.282	1.573	1.431	0.854		0.115	0.0986	0.347	1.222	1.407		3.335	10.93
2.47	0.166	0.192	0.901	1.015			0.104	0.0736	0.320	0.970			6.623	10.36
3.33	0.0958	0.0870	0.419	0.585			0.0822	0.0687	0.229	0.635			7.268	9.469
4.00	0.0648	0.0584	0.266	0.409			0.0699	0.0630	0.183	0.479			7.298	8.892
4.90	0.0384	0.0500	0.154				0.0534	0.0470	0.135				7.724	8.202

Table VI. $^{+}\sigma_{high}$ is obtained using CBX. * = corrected for pseudoresonances.

TABLE VII

Spin Weighted Partial and Total 1s-2s Cross-Sections for Excitation of O^{7+} (units 10^{-4} πa_o^2)

	SINGLET						TRIPLET							
x	L=0	L=1	L=2	L=3	L=4	L=5	L=0	L=1	L=2	L=3	L=4	L=5	$^{+}\sigma_{high}$	σ_{total}
1.04	0.269	0.466	0.0121	0.0078	0.00054	0.000011	0.0033	0.0785	0.115	0.0013	0.00032	0.000028	0.000003	0.954
1.07	0.253	0.444	0.0076	0.0084	0.00070	0.000053	0.0033	0.0763	0.119	0.0019	0.00046	0.000040	0.000006	0.915
1.20	0.195	0.473	0.0046	0.00084	0.00096	0.00011	0.0071	0.0847	0.125	0.0078	0.00031	0.00015	0.000048	0.900
1.33	0.155*	0.352	0.0076	0.0017	0.00099	0.00026	0.0082	0.0974	0.129	0.0108	0.00046	0.00024	0.00013	0.764*
1.56	0.122*	0.283	0.0174	0.00018	0.00045		0.0119	0.0705	0.113	0.0231	0.0016		0.0013	0.645*
2.00	0.0804	0.198	0.0326	0.0014	0.00013		0.0174	0.0590	0.0850	0.0298	0.0041		0.0030	0.510
2.45	0.0486	0.139	0.0386	0.0073			0.0155	0.0545	0.0676	0.0346			0.0196	0.425
3.13	0.0343	0.0882	0.0370	0.0100			0.0153	0.0498	0.0563	0.0447			0.0275	0.363
4.00	0.0213	0.0477	0.0310				0.0140	0.0440	0.0470				0.0348	0.289
4.69	0.0160	0.0421•	0.0269•				0.0122	0.0407	0.0517				0.0876	0.277

Table VII. $^{+}\sigma_{high}$ is obtained using CBX. * = corrected for pseudoresonances. • = obtained using CBX.

TABLE VIII

Spin Weighted Partial and Total 1s-2p Cross-Sections for Excitation of O^{7+} (units $10^{-4}\ \pi a_o^2$)

	SINGLET						TRIPLET							
x	L=0	L=1	L=2	L=3	L=4	L=5	L=0	L=1	L=2	L=3	L=4	L=5	$^{+}\sigma_{high}$	σ_{total}
1.04	0.228	0.392	2.041	0.638	0.0837	0.0079	0.0243	0.0670	0.0629	0.490	0.156	0.0196	0.0024	4.213
1.07	0.211	0.357	1.858	0.703	0.101	0.0118	0.0310	0.0640	0.0677	0.498	0.187	0.0294	0.0050	4.124
1.20	0.205	0.314	1.624	0.868	0.169	0.0347	0.0340	0.0637	0.0850	0.524	0.295	0.0848	0.0310	4.332
1.33	0.160*	0.235	1.211	0.660	0.217	0.0613	0.0355	0.0415	0.0989	0.512	0.370	0.146	0.0856	3.834*
1.56	0.125*	0.160	0.825	0.611	0.265		0.0418	0.0467	0.109	0.472	0.442		0.584	3.602*
2.00	0.0800	0.0800	0.498	0.463	0.280		0.0473	0.0360	0.111	0.382	0.452		1.089	3.518
2.45	0.0485	0.0610	0.293	0.342			0.0365	0.0346	0.107	0.311			1.880	3.114
3.13	0.0334	0.0388	0.163	0.160			0.0281	0.0310	0.0740	0.225			2.305	3.058
4.00	0.0186	0.0300	0.0808				0.0218	0.0260	0.0411				2.610	2.828
4.69	0.0135	0.0112*	0.0557*				0.167	0.0116	0.0448				2.486	2.640

Table VIII. $^{+}\sigma_{high}$ is obtained using CBX. * = corrected for pseudoresonances. • = values obtained using CBX.

TABLE IX

Correction for Pseudoresonances

	1s→2s		1s→2p	
x	σ(uncorrected)	σ(corrected)	σ(uncorrected)	σ(corrected)
		Z = 6		
1.33	0.413	0.502	0.565	0.534
1.40	0.208	0.459	0.564	0.483
1.43	9.537	0.440	3.082	0.460
1.50	0.520	0.393	0.386	0.423
1.60	0.377	0.327	0.362	0.379
1.70	0.285	0.263	0.346	0.352
		Z = 8		
1.33	0.142	0.155	0.163	0.160
1.40	0.0457	0.142	0.172	0.149
1.56	0.131	0.122	0.111	0.125
1.70	0.0121	0.106	0.126	0.107

TABLE IX. The ^1S spin weighted partial cross sections ($10^{-4}\ \pi a_o^2$) for C^{5+} (Z=6) and O^{7+} (Z=8), are shown as directly calculated (uncorrected), and as obtained from the K matrix fitting procedure (corrected) discussed in Section II.E.

TABLE X

Spin Weighted Partial Elastic Cross Sections for C^{5+} (units 10^{-3} πa_o^2)

	SINGLET						TRIPLET					
x	L=0	L=1	L=2	L=3	L=4	L=5	L=0	L=1	L=2	L=3	L=4	L=5
1.01	0.375	0.0015	0.0027	0.00087	0.00018	0.000072	4.680	2.200	0.170	0.0116	0.0012	0.00014
1.07	0.358	0.00088	0.0021	0.00088	0.00019	0.000077	4.326	2.056	0.167	0.0122	0.0013	0.00016
1.17	0.318	0.0011	0.0029	0.00095	0.00021	0.000084	3.810	1.852	0.163	0.0135	0.0015	0.00019
1.20	0.317	0.0015	0.0018	0.0020	0.00022	0.000086	3.698	1.741	0.162	0.0101	0.0015	0.00020
1.33	0.300	0.0017	0.0022	0.0011	0.00024	0.000090	3.165	1.486	0.149	0.0135	0.0017	0.00026
1.50	0.252	0.0027	0.0025	0.0010	0.00025		2.659	1.271	0.144	0.0141	0.0019	
2.00	0.195	0.0076	0.0018	0.00083	0.00026		1.731	0.890	0.133	0.0156	0.0023	
2.47	0.162	0.0100	0.0014	0.00077			1.242	0.662	0.119	0.0162		
3.33	0.116	0.0158	0.0016	0.00074			0.778	0.437	0.103	0.0174		
4.00	0.100	0.0211	0.0023	0.00073			0.630	0.315	0.0879	0.0177		
4.90	0.0805	0.0287	0.0033				0.457	0.165	0.0723			

TABLE XI

Spin Weighted Partial Elastic Cross Sections for O^{7+} (units 10^{-3} πa_o^2)

	SINGLET						TRIPLET					
x	L=0	L=1	L=2	L=3	L=4	L=5	L=0	L=1	L=2	L=3	L=4	L=5
1.04	0.116	0.00084	0.00055	0.000084	0.000028	0.000014	1.383	0.711	0.0629	0.0041	0.00032	0.000032
1.07	0.113	0.00062	0.00045	0.000085	0.000029	0.000014	1.323	0.683	0.0625	0.0042	0.00034	0.000035
1.20	0.102	0.00036	0.00051	0.000064	0.000032	0.000015	1.126	0.587	0.0604	0.0044	0.00041	0.000044
1.33	0.0945	0.00022	0.00037	0.00014	0.000038	0.000017	0.973	0.493	0.0536	0.0046	0.00045	0.000056
1.56	0.0802	0.00044	0.00044	0.00013	0.000036		0.769	0.411	0.0542	0.0054	0.00059	
2.00	0.0654	0.0018	0.00032	0.00011	0.000026		0.551	0.290	0.0483	0.0061	0.0084	
2.45	0.0529	0.0029	0.00012	0.00010			0.392	0.217	0.0428	0.0070		
3.13	0.0414	0.0045	0.00036	0.000098			0.269	0.153	0.0346	0.0086		
4.00	0.0318	0.0044	0.0012				0.190	0.134	0.0296			
4.69	0.0260						0.149					

TABLE XII

Collision Strengths for C^{5+} and O^{7+}

C^{5+}			O^{7+}		
x	$\Omega_{1s\to2s}$	$\Omega_{1s\to2p}$	x	$\Omega_{1s\to2s}$	$\Omega_{1s\to2p}$
1.33	1.719(-2)	0.843(-1)	1.33	0.975(-2)	0.490(-1)
1.50	1.693	0.917	1.56	0.966	0.551
2.00	1.653	1.181	2.00	0.979	0.676
2.47	1.785	1.382	2.45	1.000	0.732
3.33	1.805	1.703	3.13	1.091	0.919
4.00	1.955	1.921	4.00	1.110	1.086
4.90	2.112	2.170	4.69	1.247	1.189
6.06	2.283	2.408	5.33	1.276	1.279
8.17	2.322	2.776	9.80	1.319	1.708
10.0	2.344	3.027	17.15	1.353	2.105
14.84	2.373	3.637	24.50	1.362	2.350
20.00	2.394	3.890			

Table XII. The numbers in parenthesis indicate the power of 10 by which all numbers in the column are multiplied. Values of Ω for $x \geq 5$ are obtained using the CBX approximation.

TABLE XIII

Coefficients in the Fit to the Collision Strengths, Eq. (4 . 2)

	C^{5+}		O^{7+}	
Coef	1s→2s	2s→2p	1s→2s	1s→2p
a	0.0	1.259(-1)	0.0	7.302(-1)
b	2.730(-2)	1.044(-2)	1.521(-2)	4.456(-2)
c	-3.778(-2)	1.717(-2)	-1.812(-2)	5.664(-4)
d	3.273(-2)	4.368(-2)	1.449(-2)	3.981(-3)

Table XIII. The numbers in parenthesis indicate the power of 10 by which the number is multiplied.

TABLE XIV

Energies and Widths of Scattering Resonances Between the n=2 and n=3 Thresholds for Z=6 and Z=8

	^1S		^1P		^1D		^1F		^1G	
	x_{12}	Γ	x_{12}	Γ	x_{12}	Γ	x_{12}	Γ	x_{12}	Γ
					Z = 6					
a	1.05832	.0095	1.06373	.0286	1.06129	.0129	1.07421	.024	1.07348	.047
b	1.05832	.0095	1.06369	.0280						
a	1.06949	.0385	1.08160	.0081	1.06894	.0226	1.12372	.0027	1.12439	.0199
b	1.06945	.0386	1.08117	.0078						
a			1.12116	.0171	1.07889	.0080	1.12689	.0110	1.12891	.0042
b	1.08952	.00057								
a	1.11775	.0060	1.13056	.0037	1.11938	.0068				
b	1.11773	.0060								
a	1.12492	.0203			1.12414	.0125				
b	1.12472	.0196								
					Z = 8					
a	1.05311	.0100	1.05730	.0308	1.05536	.0132	1.06564	.0279	1.06501	.054
b	1.05311	.0100	1.05727	.0306						
a	1.06185	.0426	1.07144	.0089	1.06129	.0250	1.11848	.0029	1.11903	.0221
b	1.06180	.0418	1.07114	.0087						
a			1.11654	.0200	1.06926	.0090	1.12120	.0136	1.12301	.0061
b	1.07754	.00051								
a	1.11388	.0070	1.12424	.0041	1.11518	.0082				
b	1.11388	.0066								
a	1.11958	.0230			1.11888	.0139				
b	1.11945	.0224								

Table XIV (cont'd)

	^3S		^3P		^3D		^3F		^3G	
					Z = 6					
	x_{12}	Γ	x_{12}	Γ	x_{12}	Γ	x_{12}	Γ	x_{12}	Γ
a	1.115754	.000097	1.05908	.0075	1.06607	.0019	1.06457	.000065	1.12427	.00087
b			1.05908	.0074						
a	1.120529	.00034	1.07057	.00307						
b			1.07049	.00308						
a			1.11816	.0041						
b										
a			1.12493	.0012						
					Z = 8					
a	1.112344	.00011	1.05368	.0077	1.059075	.0020	1.057923	.000093	1.11893	.00096
b			1.05368	.0075						
a	1.116004	.00038	1.06252	.00319						
b			1.06247	.00316						
a			1.11419	.0036						
b										
a			1.11948	.0013						

Table XIV. Energies are measured in terms of the scaled variable x; widths are in Rydbergs. Rows labelled a are the present results, rows labelled b contain the results of Ho [42].

TABLE XV

Spin Weighted Partial Cross Sections for Excitation of C^{5+} (Units 10^{-4} πa_o^2) Between the n=2 and n=3 Thresholds Using the 6s-5p-2d-1f Set

[a]

L=0	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.010	0.800	0.790	0.0085	0.0758
1.030	0.745	0.692	0.0064	0.0730
1.050	0.661	0.727	0.0090	0.0790
1.0580	1.004	1.450	0.0130	0.0835
1.0582	6.520	8.261	0.0130	0.0835
1.05825	9.509	12.134	0.0131	0.0837
1.0585	9.778	11.78	0.0131	0.0837
1.0590	3.036	3.462	0.0130	0.0830
1.06253	1.008	1.003	0.0117	0.0825
1.06254	1.008	1.003	0.0117	0.0825
1.06255	1.004	0.997	0.0117	0.825
1.0680	0.835	0.789	0.105	0.800
1.0690	0.995	0.546	0.0101	0.0780
1.0695	1.144	0.358	0.0092	0.0751
1.06955	1.182	0.339	0.0090	0.0750
1.070	1.136	0.476	0.0090	0.0750
1.072	0.868	0.776	0.0115	0.0800
1.080	0.742	0.729	0.0134	0.0836
1.090	0.681	0.775	0.0115	0.0839
1.10	0.686	0.661	0.0112	0.0850
1.11249	0.546	0.529	0.0126	0.0863
1.1155	0.403	0.363	0.0112	0.0817
1.11575	0.373	0.333	0.142	0.111
1.11580	0.371	0.336	0.0236	0.118
1.1160	0.330	0.278	0.0146	0.0900
1.1175	0.674	1.062	0.0138	0.0886
1.1177	9.676	13.040	0.0135	0.0884
1.1180	4.904	6.075	0.0133	0.0860
1.1185	1.809	2.118	0.0130	0.0845
1.1205	0.945	0.981	0.0109	0.0834

L=0	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.12055	0.915	0.937	0.0194	0.0823
1.1206	0.907	0.926	0.0141	0.0872
1.1207	0.878	0.900	0.0130	0.0874
1.1245	0.836	0.600	0.0121	0.0866
1.12495	1.275	0.415	0.0120	0.0860
1.1250	1.088	0.327	0.0120	0.0860
1.1255	0.866	0.629	0.0120	0.0856
1.140	0.563	0.527	0.0115	0.0863
1.160	0.530	0.440	0.0109	0.0856

[b]

L=1	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.01	1.249	1.246	0.401	0.234
1.03	1.194	1.161	0.385	0.213
1.05	1.116	1.010	0.266	0.164
1.058	0.928	0.684	0.0826	0.0247
1.059	0.818	0.598	2.709	5.607
1.0591	0.830	0.593	5.552	9.442
1.0592	0.804	0.576	4.810	6.901
1.0594	0.788	0.553	2.285	2.629
1.0632	0.210	2.336	0.481	0.278
1.0642	3.563	9.359	0.457	0.256
1.0647	2.844	5.940	0.449	0.248
1.0704	1.404	1.731	0.394	0.234
1.0705	1.400	1.729	0.397	0.231
1.0706	1.462	1.723	0.423	0.118
1.0707	1.390	1.707	0.440	0.174
1.0811	0.728	2.639	0.400	0.186
1.0813	0.554	3.770	0.400	0.186
1.0815	0.724	7.191	0.399	0.186
1.0817	2.596	4.827	0.399	0.186
1.090	1.242	1.170	0.377	0.190
1.1181	0.797	0.520	3.240	6.389
1.11815	0.845	0.517	6.285	11.02
1.1182	0.787	0.506	6.401	9.793
1.1183	0.776	0.491	3.124	3.926
1.1210	0.735	5.000	0.454	0.248

L=1	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.12117	2.554	10.41	0.431	0.240
1.1212	2.940	11.168	0.448	0.241
1.1215	3.539	10.380	0.439	0.934
1.12478	1.369	1.709	0.405	0.177
1.12480	1.367	1.705	0.402	0.181
1.12483	1.364	1.698	0.397	0.186
1.12485	1.362	1.692	0.394	0.190
1.12488	1.359	1.698	0.388	0.198
1.12495	1.420	1.675	0.390	0.171
1.1301	0.900	1.950	0.368	0.169
1.1302	0.820	2.200	0.368	0.169
1.1303	0.710	2.699	0.367	0.168
1.1304	0.541	3.932	0.367	0.168
1.1306	2.794	6.987	0.367	0.168
1.1307	2.348	1.600	0.381	0.183
1.140	1.212	1.188	0.368	0.170
1.160	1.137	1.105	0.353	0.154

c

L=2	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.01	0.203	6.860	0.489	0.498
1.03	0.120	6.333	0.427	0.309
1.05	0.0590	5.363	0.382	0.219
1.0612	12.61	36.49	0.332	0.181
1.0614	11.96	53.93	0.330	0.180
1.0616	5.898	37.12	0.328	0.179
1.06604	0.253	6.693	6.773	13.80
1.06607	0.253	6.712	15.85	26.20
1.06610	0.252	6.732	12.37	17.15
1.0688	2.132	4.830	0.433	0.233
1.0692	1.538	8.652	0.424	0.225
1.0696	0.619	8.847	0.424	0.221
1.07875	4.930	12.24	0.388	0.194
1.07880	6.652	15.97	0.388	0.194
1.07888	8.868	22.92	0.376	0.191

L=2	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.07890	8.857	23.84	0.388	0.193
1.07895	7.598	23.45	0.388	0.193
1.090	0.0344	5.528	0.369	0.192
1.11935	15.22	48.61	0.336	0.215
1.11945	13.23	59.87	0.334	0.214
1.11960	4.918	33.91	0.330	0.213
1.1241	1.780	5.000	0.427	0.260
1.1243	1.090	7.976	0.422	0.257
1.1245	0.453	7.903	0.417	0.255
1.140	0.0292	4.244	0.403	0.301
1.160	0.0310	3.523	0.444	0.441

d

L=3	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.01	0.0378	1.938	0.0023	1.471
1.03	0.0383	1.861	0.0010	1.484
1.05	0.0408	1.749	0.00090	1.501
1.0645	0.0530	1.474	0.587	3.755
1.06464	0.0529	1.471	0.227	0.787
1.06465	0.0530	1.471	0.187	0.841
1.06466	0.0530	1.471	0.158	0.890
1.0647	0.0530	1.471	0.0890	1.026
1.0737	0.570	1.210	0.0029	1.497
1.0741	0.904	6.453	0.0028	1.496
1.0745	0.461	9.702	0.0027	1.494
1.090	0.0250	1.952	0.0042	1.518
1.123184	0.0280	0.795	0.0113	1.186
1.123187	0.0279	0.792	0.0134	1.181
1.123190	0.0278	0.788	0.0159	1.175
1.12369	0.205	4.375	0.0094	1.517
1.12370	0.321	6.633	0.0110	1.560
1.12374	0.601	12.69	0.0086	1.513
1.12378	0.480	10.03	0.0082	1.509
1.12678	1.124	4.726	0.0163	1.571

L=3	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.12688	1.190	8.983	0.0162	1.572
1.12696	0.893	10.35	0.0115	1.554
1.12714	0.267	8.014	0.0093	1.546
1.140	0.0240	1.872	0.0135	1.553
1.160	0.0260	1.736	0.0180	1.560

e

L=4	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.01	0.0012	0.117	0.0053	0.328
1.03	0.0011	0.144	0.0042	0.387
1.05	0.00070	0.167	0.0032	0.449
1.0732	0.171	0.287	0.0024	0.524
1.0739	0.184	0.742	0.0024	0.526
1.0749	0.0756	0.628	0.0023	0.530
1.090	0.0043	0.300	0.0018	0.583
1.1241	0.135	0.0626	0.0205	0.326
1.1244	0.257	0.494	0.0105	1.294
1.1248	0.143	0.719	0.00080	0.802
1.12875	0.00023	0.0424	0.0017	0.693
1.12882	0.0063	0.415	0.0017	0.693
1.12890	0.0460	2.492	0.0017	0.693
1.1290	0.0486	2.428	0.0013	0.726
1.140	0.0052	0.432	0.0012	0.768
1.160	0.0043	0.458	0.0012	0.847

TABLE XV. Values of X were conveniently chosen in order to trace resonances and provide the background as well.

TABLE XVI

Spin Weighted Partial Cross Sections for Excitation of O^{7+} (Units 10^{-4} πa_o^2) Between the n=2 and n=3 Thresholds Using the 6s-5p-2d-1f Set

[a]

L=0	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.01	0.296	0.216	0.0036	0.0504
1.03	0.260	0.189	0.0036	0.0509
1.05	0.204	0.134	0.0036	0.0508
1.05235	0.0182	0.0013	0.0036	0.0507
1.0524	0.0122	0.0025	0.0039	0.0515
1.05245	0.0070	0.0063	0.0039	0.0521
1.0529	0.639	1.146	0.0035	0.0520
1.0530	2.256	3.487	0.0037	0.0509
1.05308	6.188	8.686	0.0037	0.0508
1.0535	1.368	1.616	0.0032	0.0510
1.054	0.656	0.705	0.0032	0.0512
1.061	0.299	0.227	0.0032	0.0520
1.0618	0.385	0.117	0.0036	0.0524
1.06188	0.386	0.115	0.0037	0.0549
1.062	0.389	0.129	0.0032	0.0525
1.063	0.299	0.237	0.0033	0.0528
1.07755	0.236	0.234	0.0034	0.0530
1.09	0.242	0.186	0.0040	0.0531
1.112	0.146	0.0936	0.0041	0.0519
1.1125	0.119	0.0687	0.0052	0.0568
1.113	0.0711	0.0287	0.0047	0.0544
1.1138	1.804	2.940	0.0043	0.0544
1.11386	5.992	8.695	0.0047	0.0545
1.11388	7.320	10.34	0.0046	0.0544
1.1139	7.472	10.76	0.0043	0.0545
1.11395	5.250	7.268	0.0043	0.0546
1.1140	3.194	4.250	0.0042	0.0548
1.1155	0.361	0.319	0.0052	0.0563
1.1159	0.333	0.289	0.0045	0.0537
1.1160	0.327	0.282	0.0120	0.0490

L=0	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.1165	0.308	0.261	0.0047	0.0543
1.1190	0.262	0.229	0.0042	0.0530
1.1195	0.336	0.121	0.0042	0.0536
1.1196	0.350	0.104	0.0044	0.0537
1.120	0.285	0.198	0.0042	0.0540
1.140	0.0412	0.0074	0.0058	0.0569
1.160	0.218	0.168	0.0056	0.0550

b

L=1	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.01	0.567	0.608	0.0663	0.0594
1.03	0.531	0.519	0.0708	0.0608
1.0505	0.400	0.269	0.0446	0.0491
1.0536	0.316	0.183	0.956	2.065
1.0537	0.313	0.179	2.929	5.219
1.0538	0.309	0.175	1.421	2.195
1.0570	0.223	1.794	0.113	0.0922
1.0572	0.897	4.559	0.0704	0.116
1.0576	1.800	4.429	0.108	0.0871
1.0579	1.336	2.616	0.106	0.0850
1.0624	0.538	0.553	0.0930	0.0789
1.0625	0.535	0.550	0.105	0.0639
1.0626	0.533	0.546	0.109	0.0559
1.0705	0.407	0.583	0.0688	0.0774
1.1711	0.248	1.061	0.0914	0.0659
1.07123	0.174	1.658	0.0914	0.0659
1.07132	0.156	2.817	0.0913	0.0658
1.09	0.491	0.381	0.0939	0.0748
1.1141	0.304	0.161	0.351	0.742
1.11415	0.337	0.189	1.467	3.031
1.1142	0.299	0.156	3.376	6.064
1.1143	0.294	0.149	1.023	1.465
1.1164	0.176	1.585	0.113	0.0825
1.1165	0.710	3.960	0.0740	0.107
1.1166	1.889	6.167	0.111	0.0800

L=1	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.1168	1.867	5.153	0.109	0.0783
1.11942	0.525	0.128	0.0976	0.0644
1.11944	0.524	0.535	0.0981	0.0640
1.11946	0.523	0.534	0.101	0.0605
1.11948	0.522	0.533	0.122	0.0341
1.1239	0.329	0.687	0.0921	0.0589
1.1240	0.286	0.869	0.0930	0.0582
1.1241	0.203	1.426	0.0921	0.0586
1.1242	0.241	4.895	0.0924	0.0582
1.1243	1.149	1.946	0.0910	0.0588
1.14	0.456	0.282	0.115	0.0877
1.16	0.424	0.230	0.121	0.0898

c

L=2	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.01	0.0158	2.390	0.108	0.0480
1.03	0.0117	2.131	0.109	0.0523
1.0553	6.340	18.51	0.101	0.0563
1.05545	5.841	27.78	0.101	0.0561
1.05557	2.613	16.87	0.100	0.0560
1.05906	0.566	2.211	5.570	9.245
1.05908	0.0568	2.205	10.01	14.12
1.05911	0.0570	2.196	3.565	4.129
1.0612	0.985	1.999	0.135	0.0692
1.06146	0.709	3.747	0.133	0.0681
1.06171	0.271	3.476	0.131	0.0675
1.06606	0.0168	2.163	0.114	0.0629
1.06910	1.544	3.762	0.118	0.0624
1.06917	1.814	6.632	0.117	0.0627
1.06924	5.570	12.42	0.117	0.0627
1.09	0.0054	1.734	0.115	0.0681
1.11507	3.841	10.49	0.104	0.0695
1.11512	8.270	25.48	0.0981	0.0687
1.11514	9.160	31.77	0.103	0.0693
1.11521	5.602	27.71	0.103	0.0690

L=2	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.1186	0.209	1.252	0.137	0.0842
1.11875	0.480	1.218	0.135	0.0850
1.11888	0.792	2.455	0.134	0.0867
1.140	0.0028	1.395	0.117	0.0812
1.160	0.0020	1.225	0.118	0.0867

d

L=3	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.010	0.0201	0.601	0.00031	0.477
1.030	0.0149	0.594	0.00033	0.483
1.0579	0.0121	0.513	0.705	2.631
1.0580	0.0122	0.513	0.0911	0.197
1.0581	0.0122	0.513	0.0230	0.340
1.06545	0.483	2.338	0.0023	0.489
1.06563	0.602	5.071	0.0023	0.489
1.06576	0.460	5.636	0.0023	0.489
1.090	0.0211	0.662	0.0040	0.498
1.11843	0.0389	0.551	0.0077	0.505
1.11846	0.172	3.080	0.0074	0.503
1.11848	0.342	6.738	0.0072	0.503
1.11849	0.354	7.317	0.0066	0.497
1.12112	0.636	2.670	0.0086	0.514
1.12118	0.757	4.519	0.0076	0.510
1.12125	0.636	5.656	0.0078	0.509
1.12135	0.295	4.379	0.0074	0.510
1.14	0.00041	0.701	0.0105	0.513
1.16	0.0011	0.690	0.0139	0.518

e

L=4	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.010	0.00010	0.0447	0.0027	0.130
1.03	0.000096	0.0554	0.0018	0.145
1.05	0.000035	0.0622	0.0011	0.167
1.0645	0.0533	0.0563	0.00027	0.180
1.0650	0.108	0.330	0.00027	0.180

L=4	S=0		S=1	
X	σ_{1s-2s}	σ_{1s-2p}	σ_{1s-2s}	σ_{1s-2p}
1.06545	0.0734	0.404	0.00027	0.181
1.06560	0.0580	0.372	0.00027	0.181
1.090	0.00062	0.110	0.00034	0.207
1.11880	0.0607	0.0295	0.0057	0.107
1.1190	0.133	0.243	0.0151	0.619
1.1192	0.0966	0.383	0.00096	0.310
1.12288	0.00094	0.0664	0.00021	0.238
1.12294	0.0059	0.400	0.00022	0.238
1.1230	0.0235	1.569	0.00022	0.238
1.14	0.0010	0.164	0.00033	0.263
1.16	0.00098	0.179	0.00061	0.285

TABLE XVI. Values of X were conveniently chosen in order to trace resonances and provide the background as well.

TABLE XVII

Thermally Averaged Excitation Cross-Sections for C^{5+} (units 10^{-4} πa_o^2)

T(KeV)	Ar/An	Ar/B	$\bar{\sigma}_{1s\to 2s}$	Ar/An	Ar/B	$\bar{\sigma}_{1s\to 2p}$
0.05	1.08	3.04	0.0161	1.04	2.60	0.0680
0.10	1.08	1.04	0.311	1.04	0.81	1.432
0.15	1.08	0.62	0.695	1.04	0.45	3.478
0.20	1.08	0.44	0.954	1.05	0.30	5.142
0.25	1.08	0.34	1.101	1.05	0.22	6.312
0.50	1.11	0.15	1.174	1.05	0.08	8.264
0.75	1.09	0.10	1.033	1.04	0.05	8.207
1.00	1.09	0.07	0.901	1.05	0.03	7.780
1.25	1.09	0.05	0.796	1.05	0.025	7.328
1.50	1.09	0.04	0.712	1.04	0.02	6.877
1.75	1.10	0.035	0.644	1.04	0.015	6.482
2.00	1.11	0.03	0.588	1.04	0.01	6.137

Table XVII. The ratio Ar/An measures the resonance enhancement over the background in the resonance region; the ratio Ar/B measures that region's contribution to the total cross section.

TABLE XVIII

Thermally Averaged Excitation Cross-Sections for O^{7+} (units 10^{-4} πa_o^2)

T(KeV)	Ar/An	Ar/B	$\bar{\sigma}_{1s\to 2s}$	Ar/An	Ar/B	$\bar{\sigma}_{1s\to 2p}$
0.10	1.08	2.66	0.0107	1.05	2.12	0.0463
0.15	1.08	1.41	0.0618	1.05	1.08	0.280
0.20	1.08	0.95	0.136	1.05	0.70	0.644
0.25	1.08	0.71	0.207	1.05	0.50	1.023
0.50	1.08	0.31	0.378	1.05	0.19	2.207
0.75	1.09	0.19	0.394	1.05	0.11	2.577
1.00	1.09	0.14	0.374	1.05	0.07	2.660
1.25	1.08	0.11	0.347	1.06	0.05	2.637
1.50	1.08	0.09	0.320	1.05	0.04	2.572
1.75	1.08	0.07	0.297	1.05	0.03	2.493
2.00	1.08	0.06	0.276	1.05	0.025	2.409

Table XVIII. The ratio Ar/An measures the resonance enhancement over the background in the resonance region; the ratio Ar/B measures that region's contribution to the total cross section.

FIGURE CAPTIONS

Figure I — Real part of the ^1S 1s→2s transition amplitude for electron impact excitation of C^{5+} is shown as a function of the scaled energy x (defined as the ratio of the incident energy to the n=2 state excitation threshold), in the vicinity of the pseudopole at x = 1.4306. The dark dots (connected by a light solid line as an eye guide) are the calculated points. The dashed curve is obtained by making a linear least fit to the transition amplitudes with a quadratic form in k^2; the solid line is the amplitude calculated from the K matrix fit discussed in the text (Section II.E).

Figure II — Same as Fig. I except that the imaginary part of the 1s→2s transition amplitude is shown.

Figure III — The ^1S 1s→2s excitation cross section for C^{5+} is shown as computed from the transition amplitudes shown in Figs. I and II. The three curves have the same significance as in Fig. I.

Figure IV — The ^1S 1s-2p excitation cross-section for C^{5+} as a function of the scaled energy x, is shown as computed following a similar procedure as for the 1s→2s cross section (Fig. III). The different curves shown have the same significance as in Fig. I.

Figure V Collision strength for the 2s excitation of C^{5+}. Curves are: PS, present pseudostate calculation (from Eq. (4.2) with coefficients listed in Table XIII); 3cc, three state close coupling by Robb; CBX, Coulomb Born with exchange by Mann; IZH, infinite Z hydrogenic by Sampson; DW, distorted wave by Mann; CB, Coulomb Born by Mann. The dark triangles (▲) show a few values by a second order potential calculation by Bransden and Noble.

Figure VI Collision strength for the 2s excitation of O^{7+}. Curves are: PS, present pseudostate calculation (from Eq. (4.2) with coefficients listed in Table XIII); CBX, Coulomb Born with exchange by Callaway; IZH, infinite Z hydrogenic by Sampson; DW, distorted wave by Mann; CB, Coulomb Born by Tully.

Figure VII Collision strength for 2p excitation of C^{5+}. Curves are: PS, present pseudostate calculations; IZH, infinite Z hydrogenic by Sampson; CB, Coulomb Born by Mann.

Figure VIII Collision strength for 2p excitation of O^{7+}. Curves are: PS, present pseudostate calculation; CB, Coulomb Born by Mann.

Figure IX The ^1P contribution to the 1s→2s excitation cross section for C^{5+} (units $10^{-4}\ \pi a_o^2$) is shown in the resonance region from x = 1.0 to x = 1.1851.

Figure X The ^1F contribution to the 1s→2s excitation cross section (units $10^{-5}\ \pi a_o^2$) for C^{5+} in the resonance region.

Figure XI The ^1D contribution to the 1s→2p excitation cross section (units $10^{-3}\ \pi a_o^2$) for O^{7+} in the resonance region.

Figure XII The ^1F contribution to the 1s→2p excitation cross section (units $10^{-4}\ \pi a_o^2$) for O^{7+} in the resonance region.

Figure XIII Cross section for 2s excitation of C^{5+} (units $10^{-4}\ \pi a_o^2$) in the resonance region from x = 1.0 to x = 1.1851.

Figure XIV Cross section for 2p excitation of C^{5+} (units $10^{-3}\ \pi a_o^2$) in the resonance region.

Figure XV Cross section for 2s excitation of O^{7+} (units $10^{-5}\ \pi a_o^2$) in the resonance region.

Figure XVI Cross section for 2p excitation of O^{7+} (units $10^{-4}\ \pi a_o^2$) in the resonance region.

Figure XVII Thermally averaged 1s→2s and 1s→2p excitation cross sections (units $10^{-4}\ \pi a_o^2$) for C^{5+} are plotted as a function of the electron temperature in KeV units. The solid curves represent

the present calculation. The dashed curves are based on the distorted wave calculation by Mann.[17]

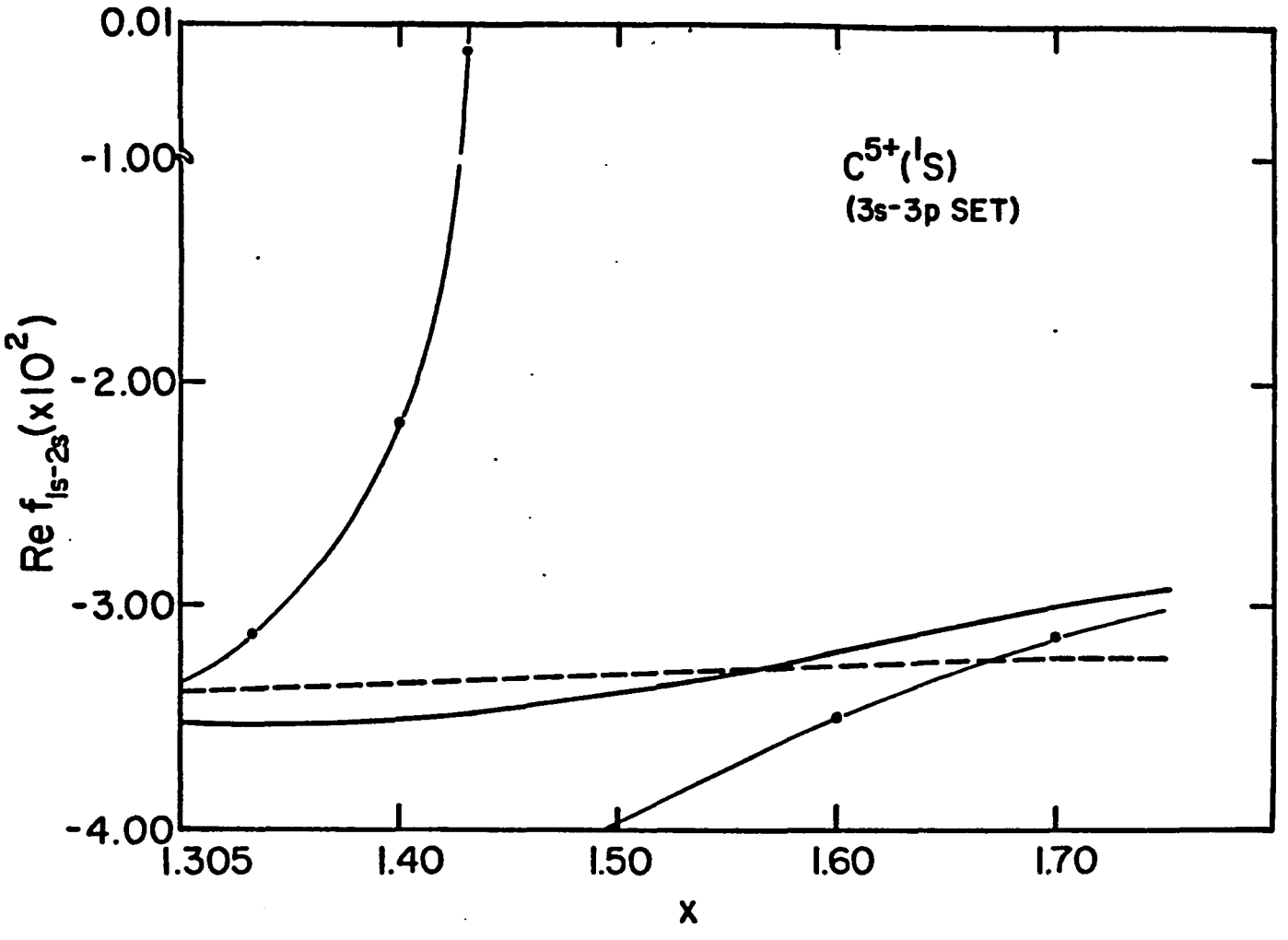
Figure XVIII Thermally averaged 1s→2s and 1s→2p excitation cross sections (units 10^{-4} πa_o^2) for O^{7+}. Curves have the same significance as in Fig. XVII.

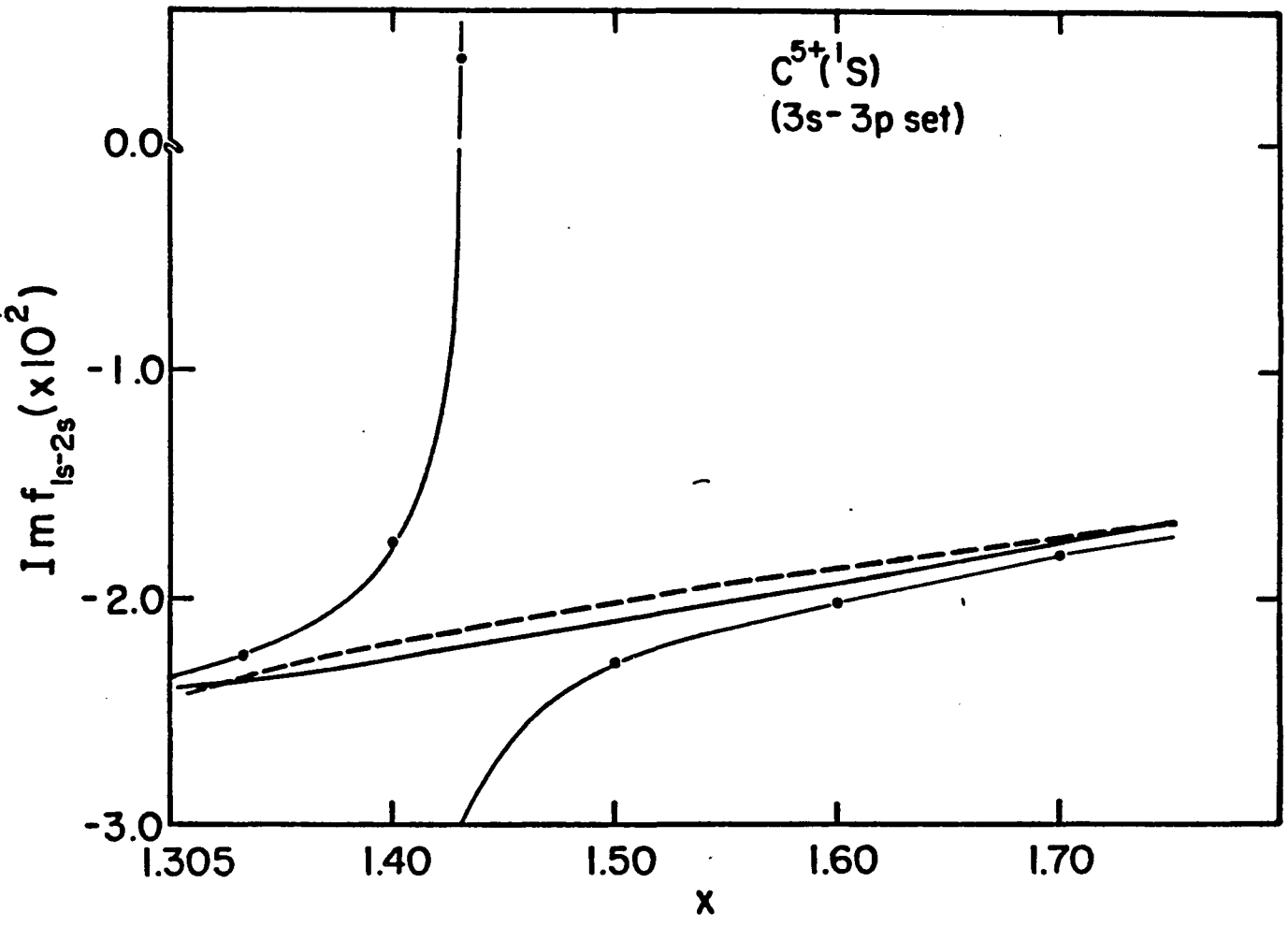
Figure XIX S wave phase shifts in radians for scattering by the static potential defined in Eq. (A.1) with Z=2, are plotted as a function of the parameter γ at k_i^2 = 1.0 and 2.0 Rydbergs.

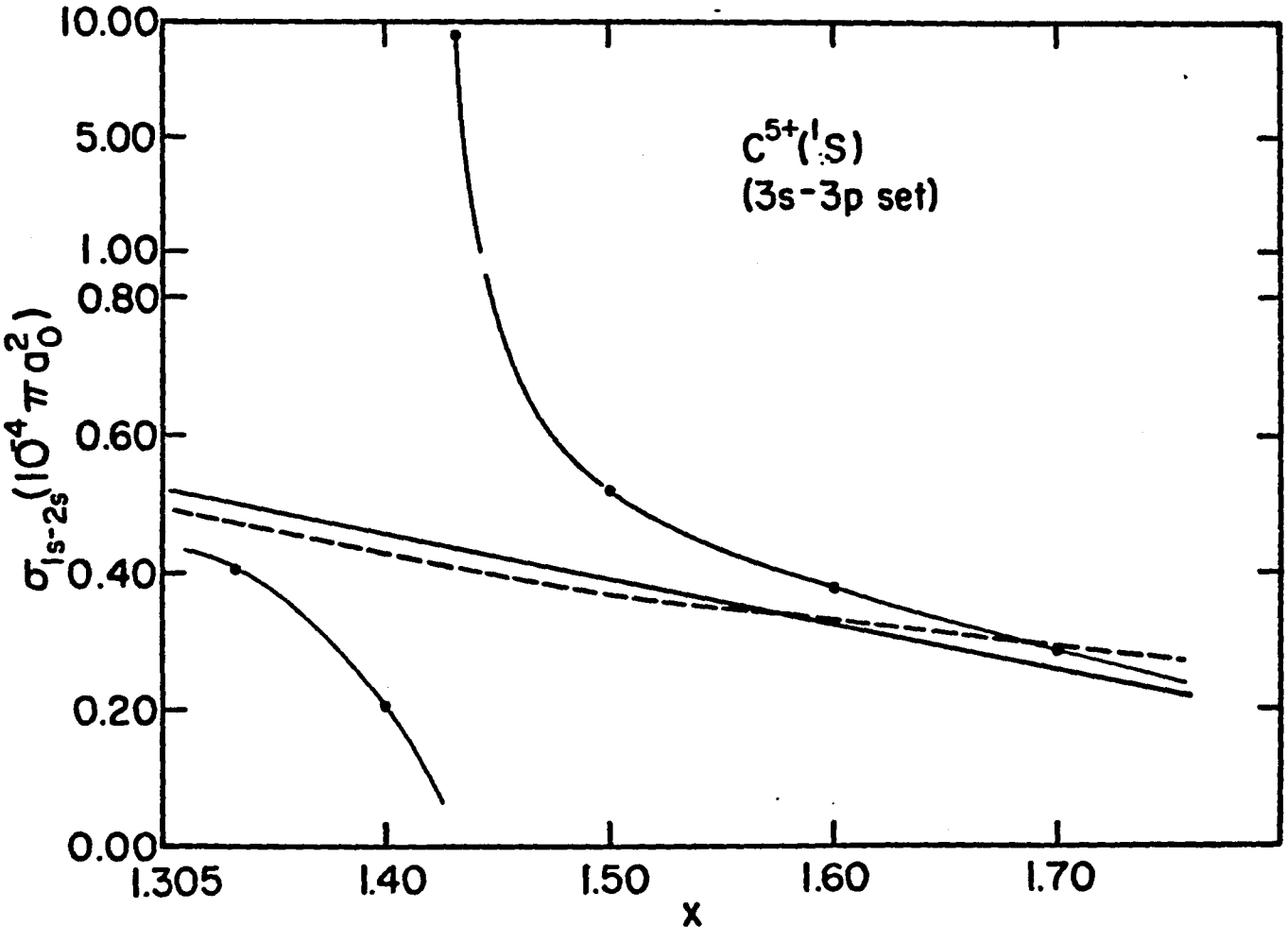
Figure XX ^1S phase shift in radians for electron scattering by C^{5+} is plotted as a function of the parameter γ at k_i^2 = 16.0 Ry.

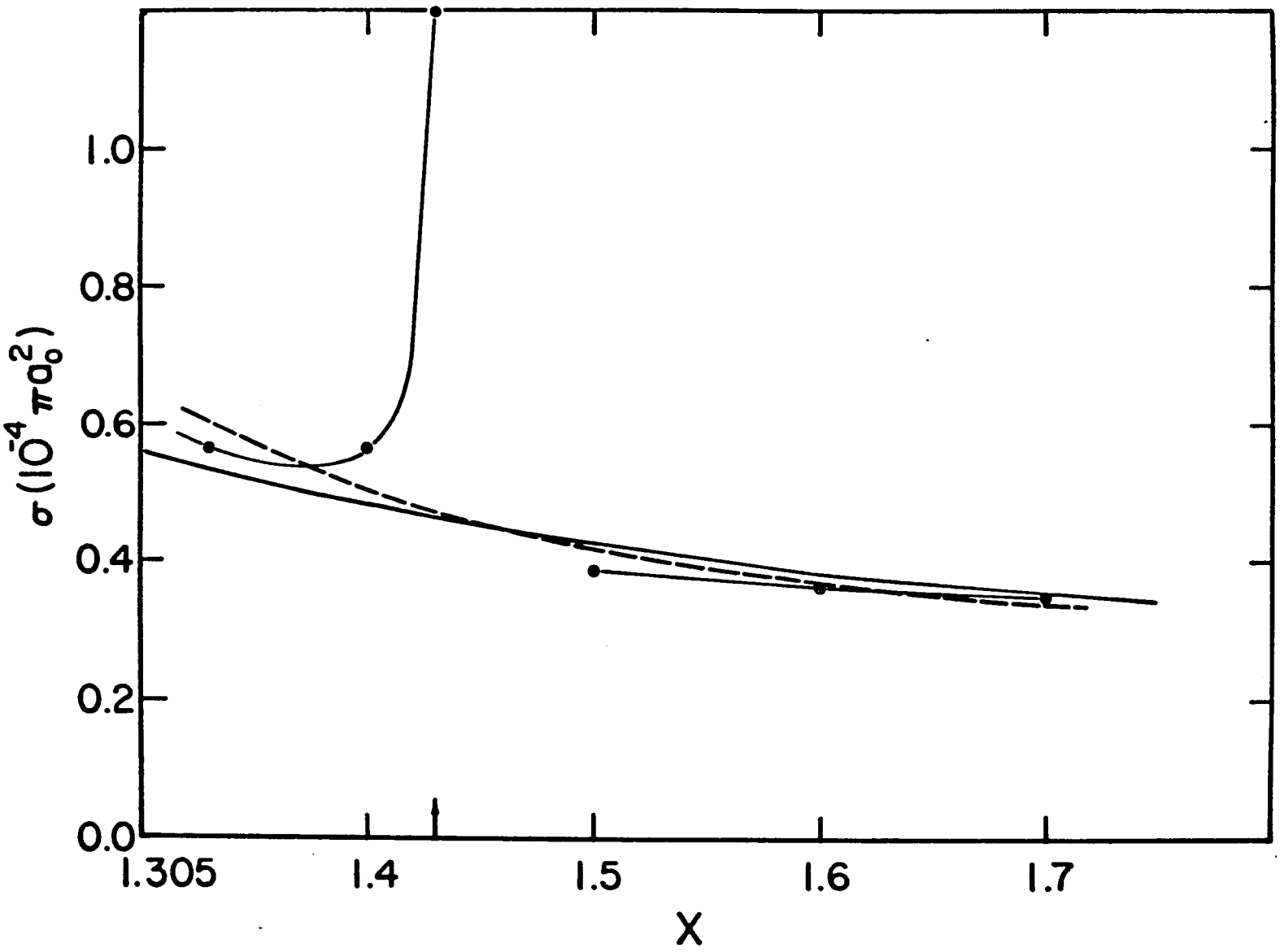
Figure XXI Same as Fig. XX except that the ^3S phase shift is shown.

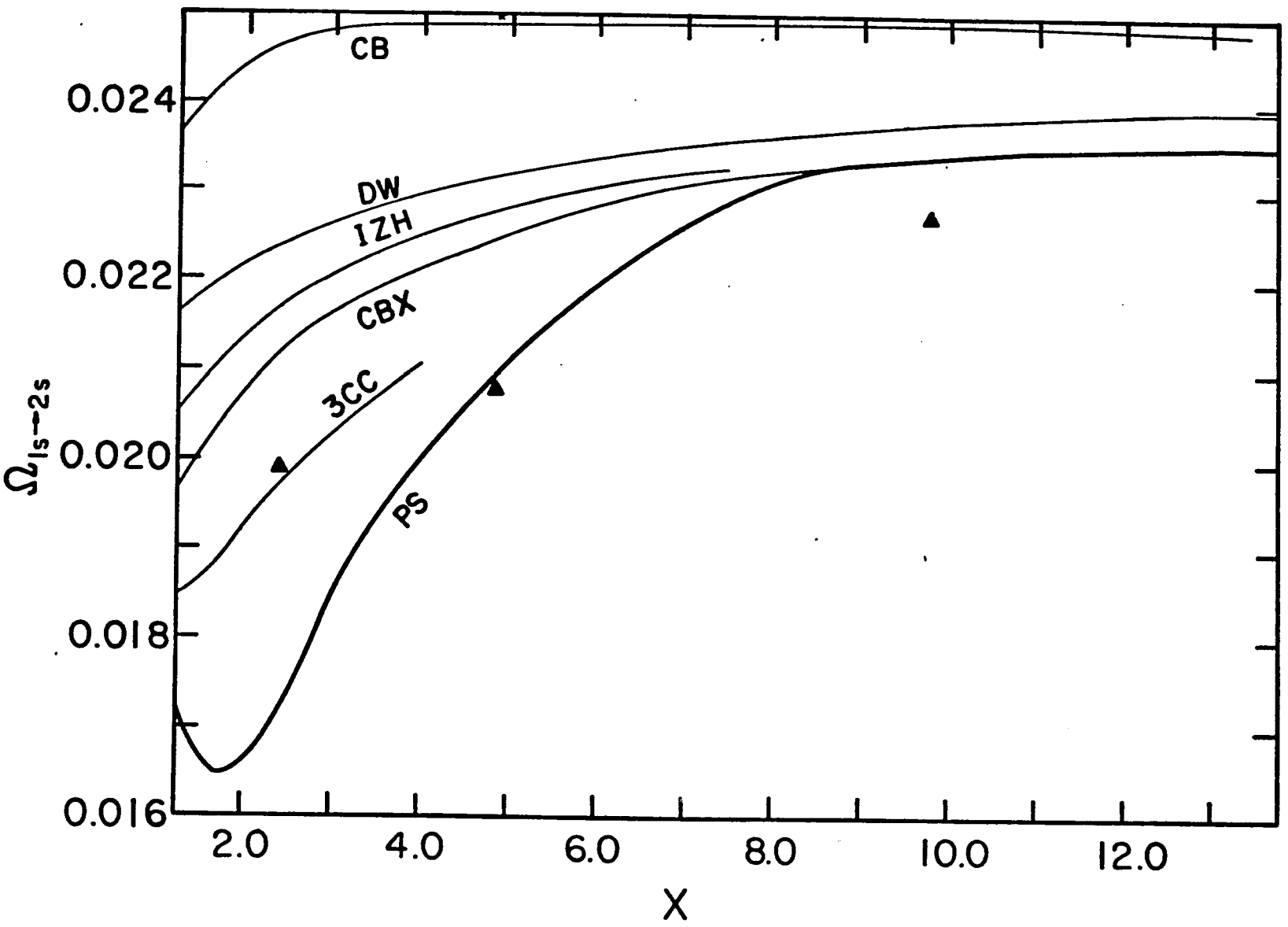
Figure XXII Partial s wave singlet and triplet eigenphase sums (in radians) for excitation of C^{5+} at x = 1.07, as a function of the parameter γ.


0.01
-1.00
-2.00
-3.00
-4.00
Re f_{1s-2s} ($\times 10^2$)
$C^{5+}(^1S)$
(3s-3p SET)
1.305
1.40
1.50
1.60
1.70
X


$C^{5+}(^1S)$
(3s - 3p set)
0.0
-1.0
-2.0
-3.0
$Im\, f_{1s-2s}(x10^2)$
1.305
1.40
1.50
1.60
1.70
x


10.00
5.00
1.00
0.80
0.60
0.40
0.20
0.00
$\sigma_{1s-2s}(10^{-4}\pi a_0^2)$
$C^{5+}(^1S)$
(3s-3p set)
1.305
1.40
1.50
1.60
1.70
X


1.0
0.8
0.6
0.4
0.2
0.0
σ (10^-4 π a_0^2)
1.305
1.4
1.5
1.6
1.7
X


CB
DW
IZH
CBX
3CC
PS
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0.022
0.020
0.018
0.016
$\Omega_{1s\to 2s}$
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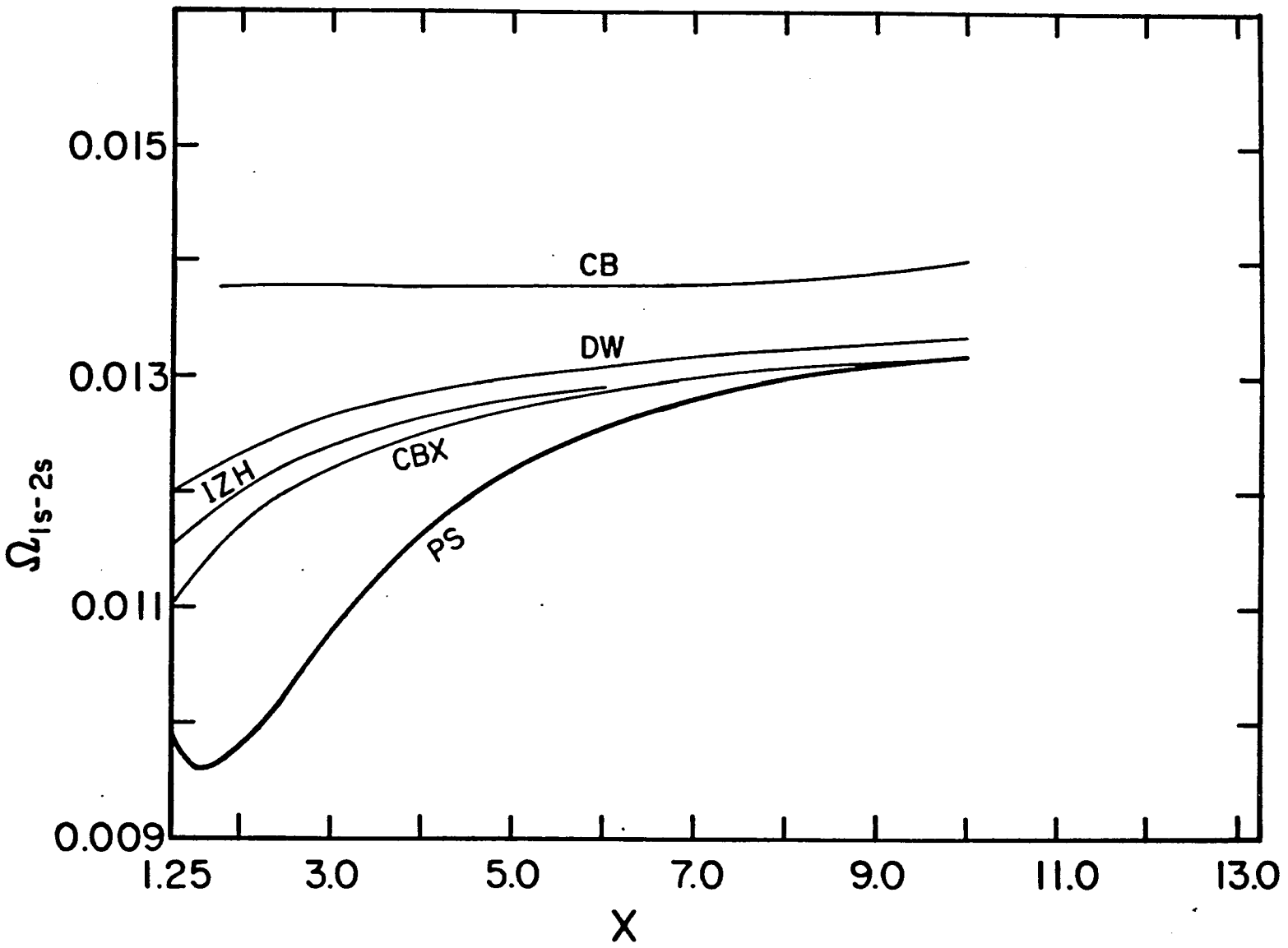
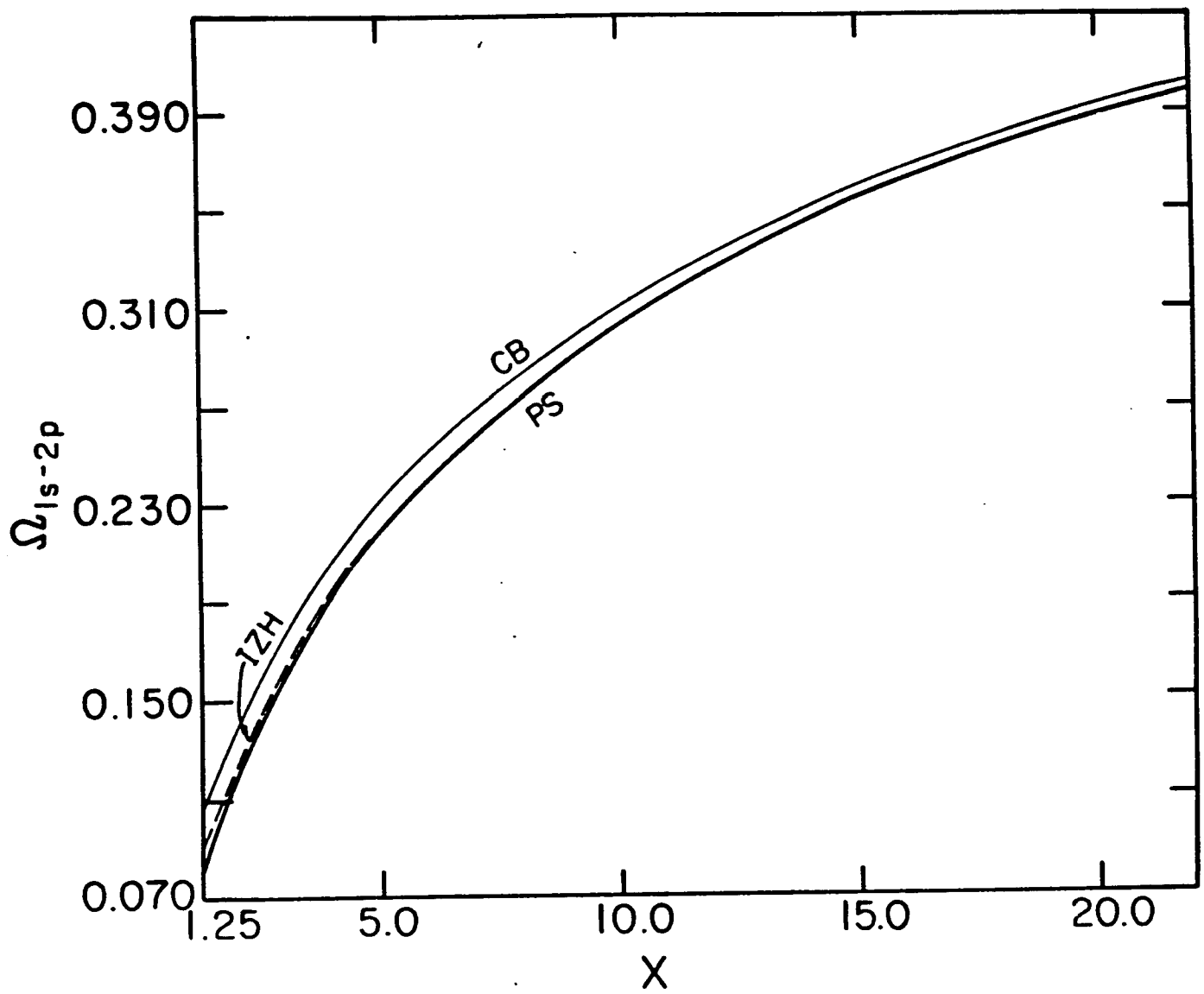
4.0
6.0
8.0
10.0
12.0
X


0.015
0.013
0.011
0.009
Ω_{1s-2s}
CB
DW
CBX
IZH
PS
1.25
3.0
5.0
7.0
9.0
11.0
13.0
X


0.390
0.310
0.230
0.150
0.070
Ω_{1s-2p}
CB
PS
IZH
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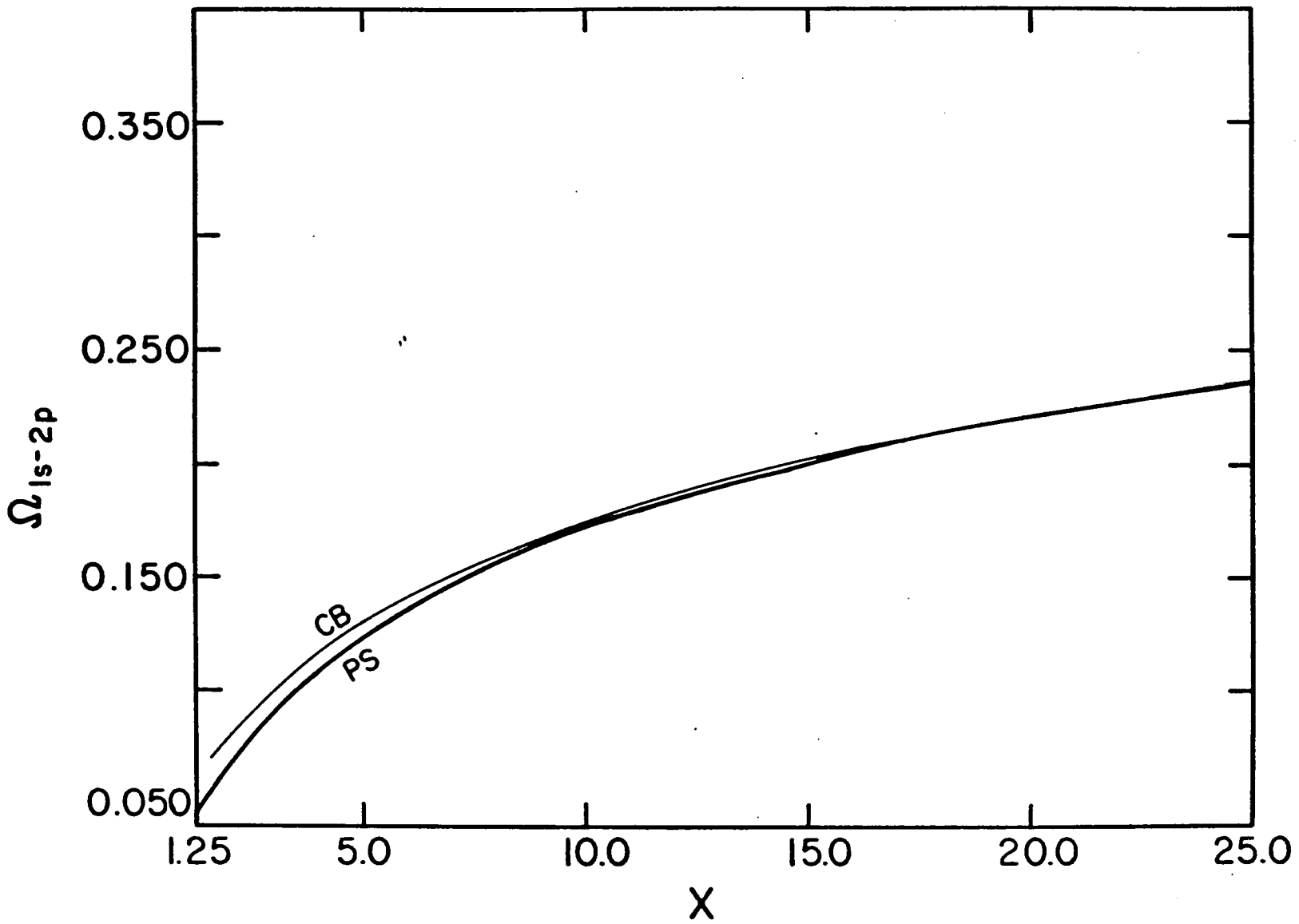
5.0
10.0
15.0
20.0
X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0.250
0.150
0.050
Ω_{1s-2p}
CB
PS
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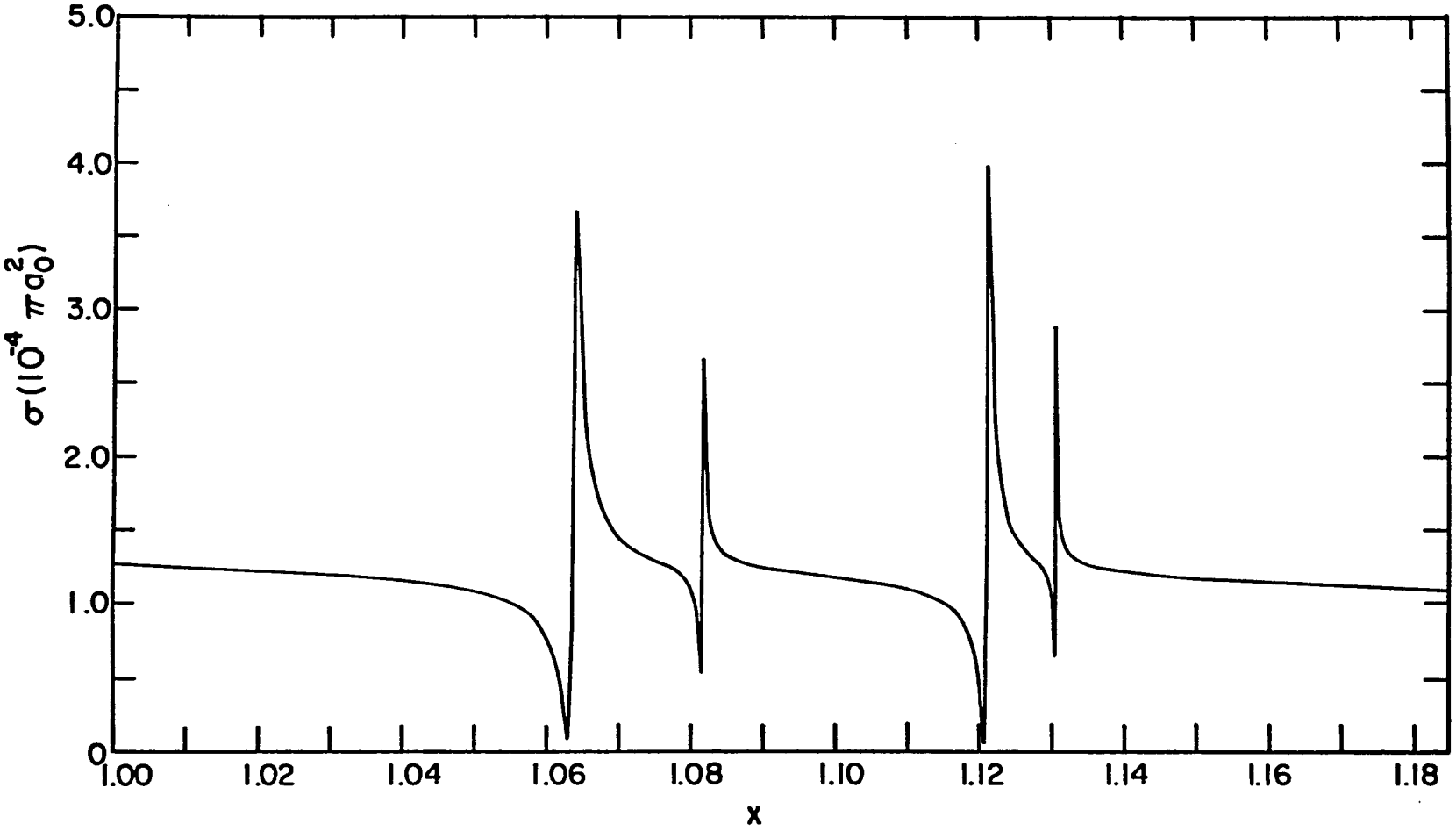
5.0
10.0
15.0
20.0
25.0
X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4.0
3.0
2.0
1.0
0
σ(10^-4 πa_0^2)
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1.02
1.04
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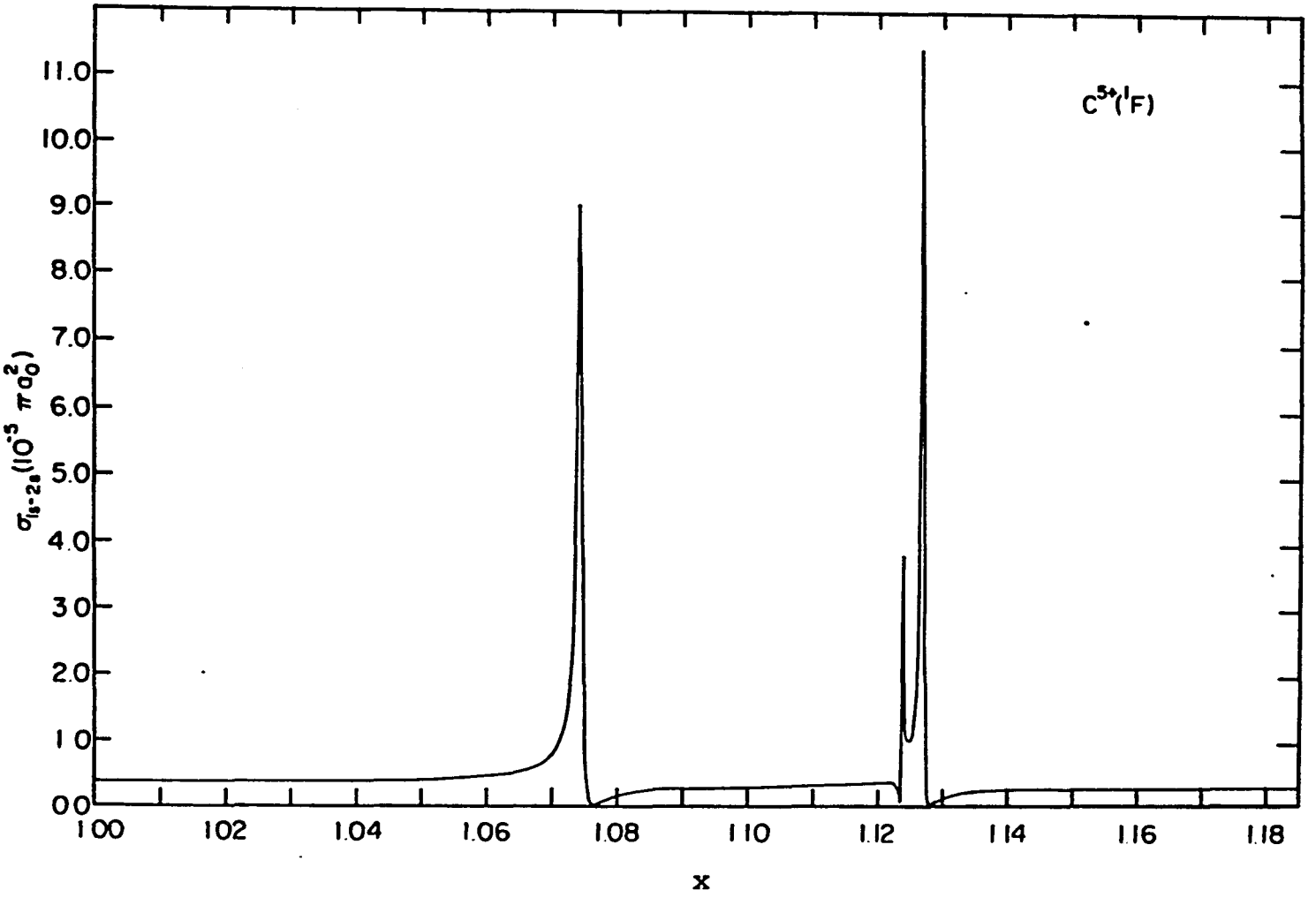
1.08
1.10
1.12
1.14
1.16
1.18
x


$C^{5+}(^1F)$
$\sigma_{1s-2s}(10^{-3}\ \pi a_0^2)$
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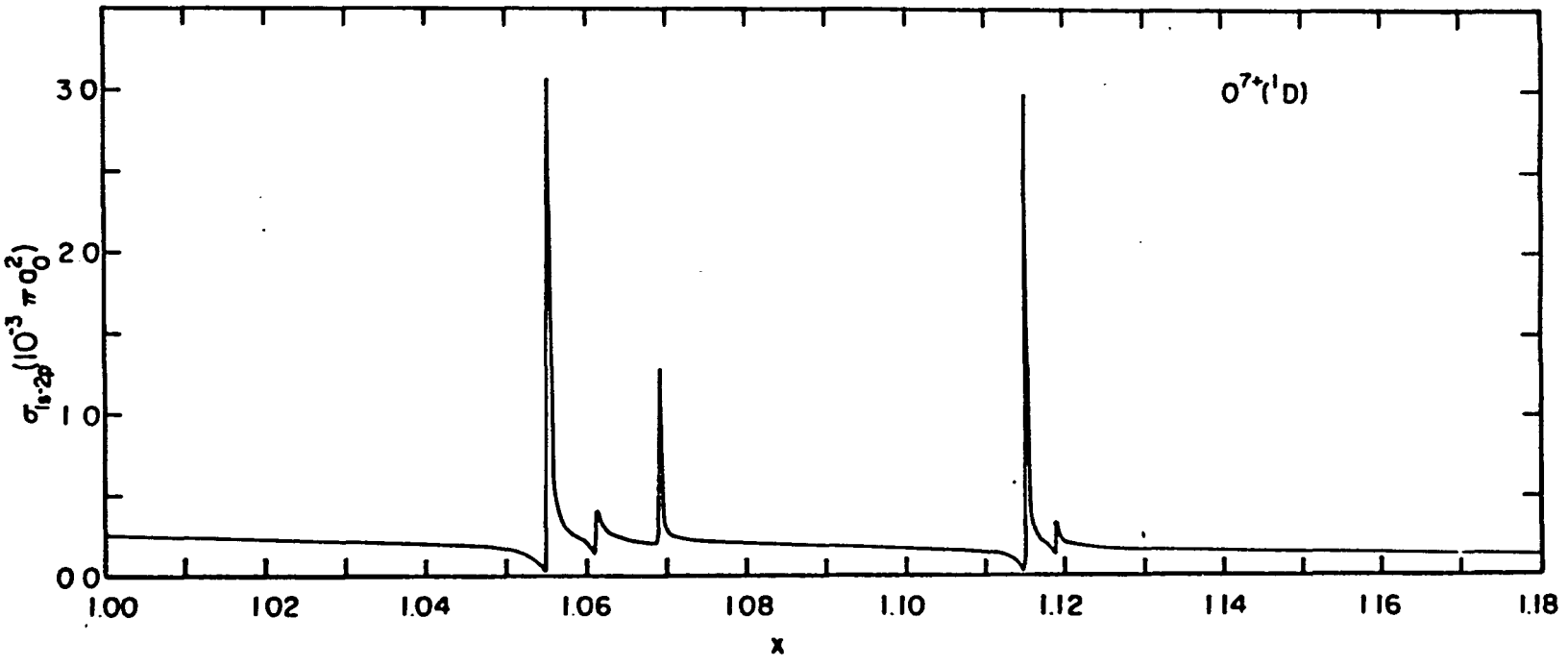
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.00
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
1.18
x


$O^{7+}(^1D)$
$\sigma_{1s\text{-}2p}(10^{-3}\pi a_0^2)$
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2 0
1 0
0 0
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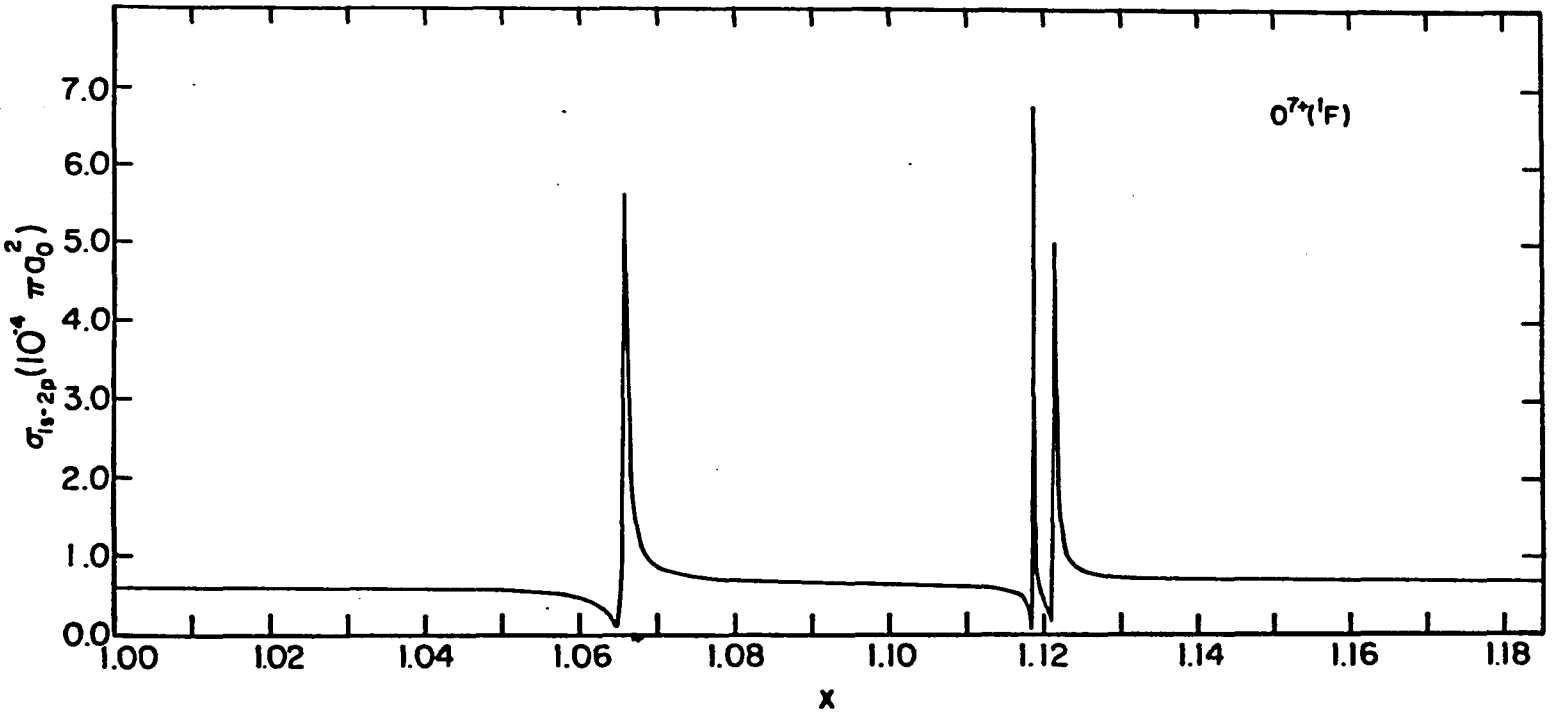
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
1.18
x


$O^{7+}(^1F)$
$\sigma_{1s-2p}(10^{-4}\ \pi a_0^2)$
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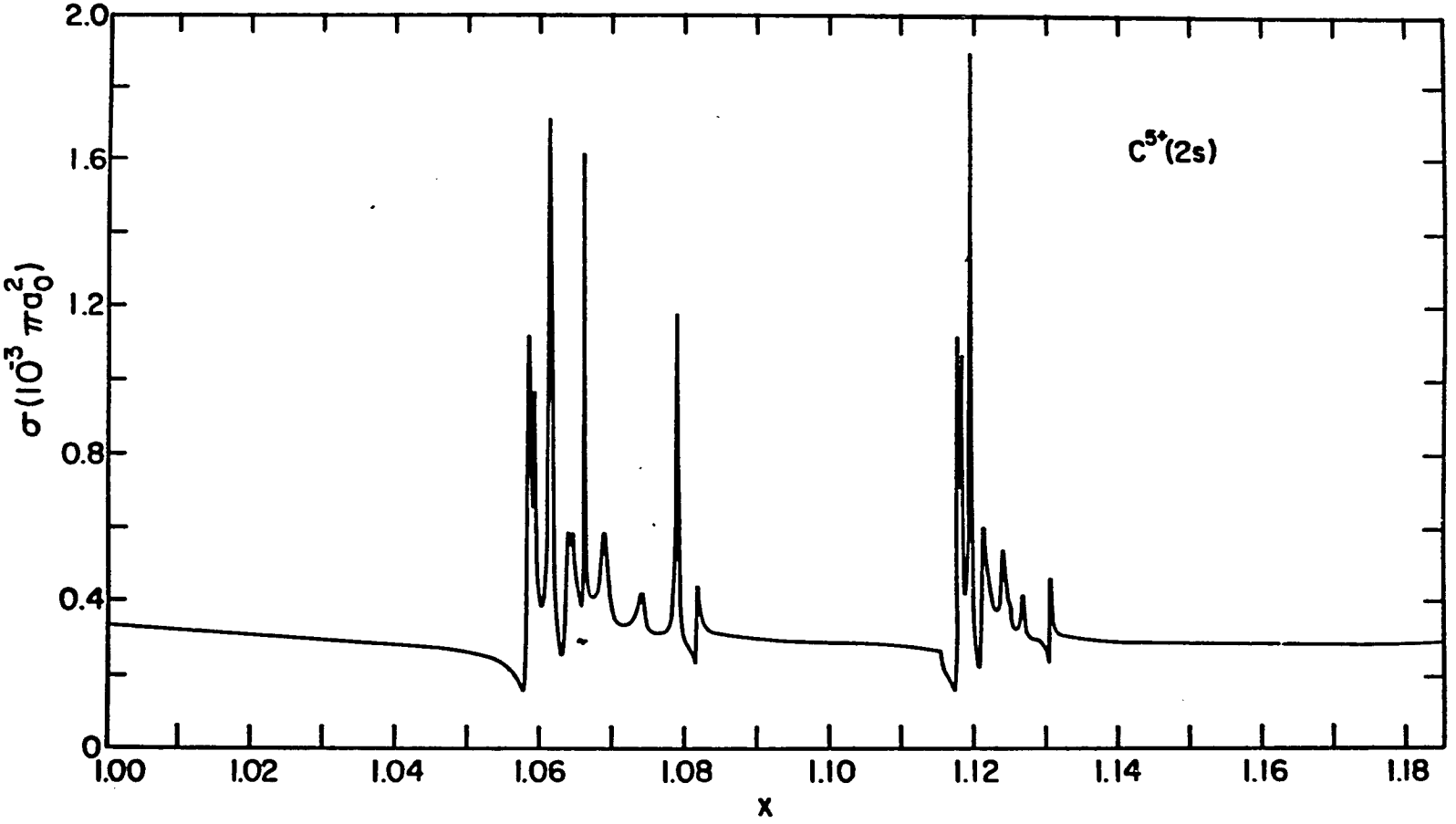
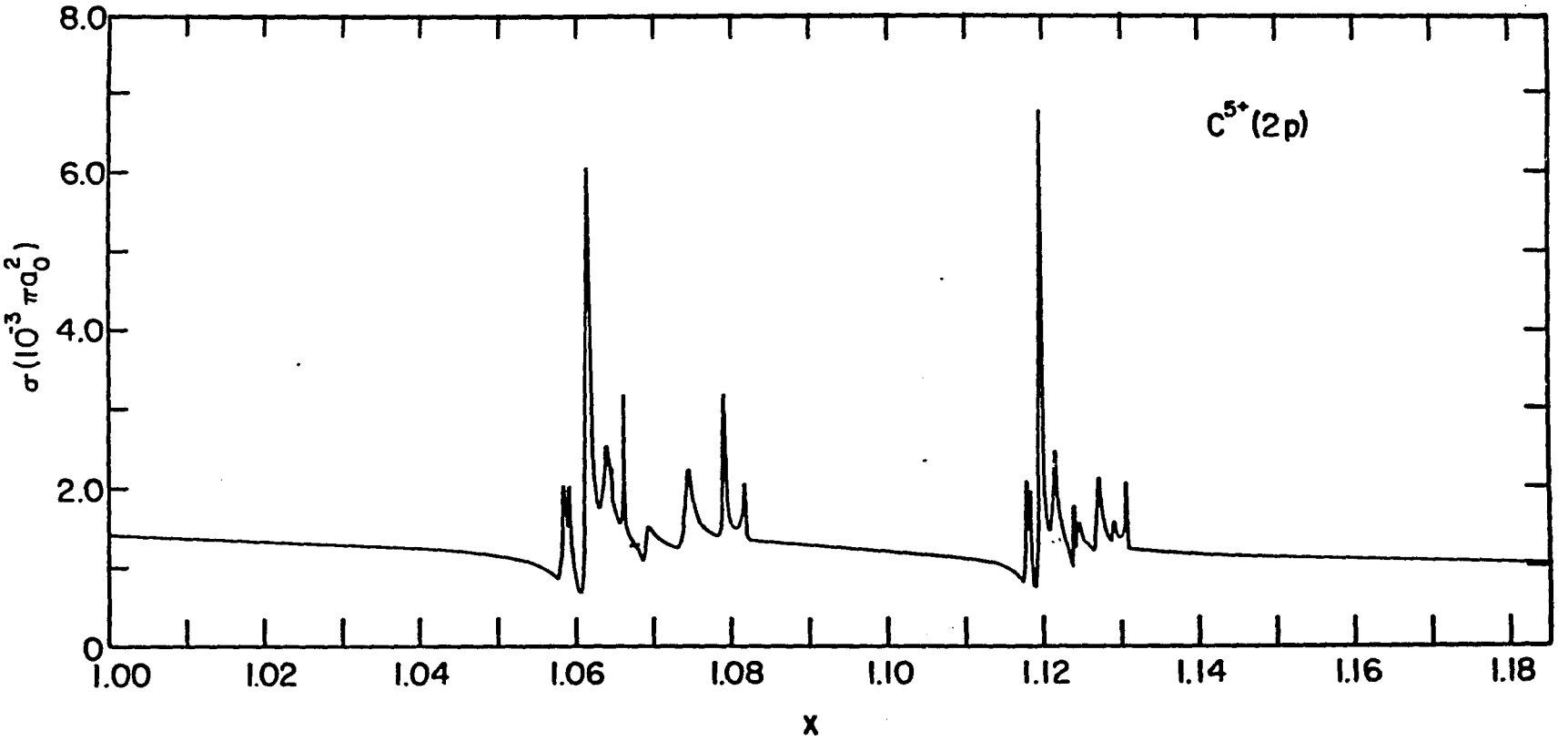
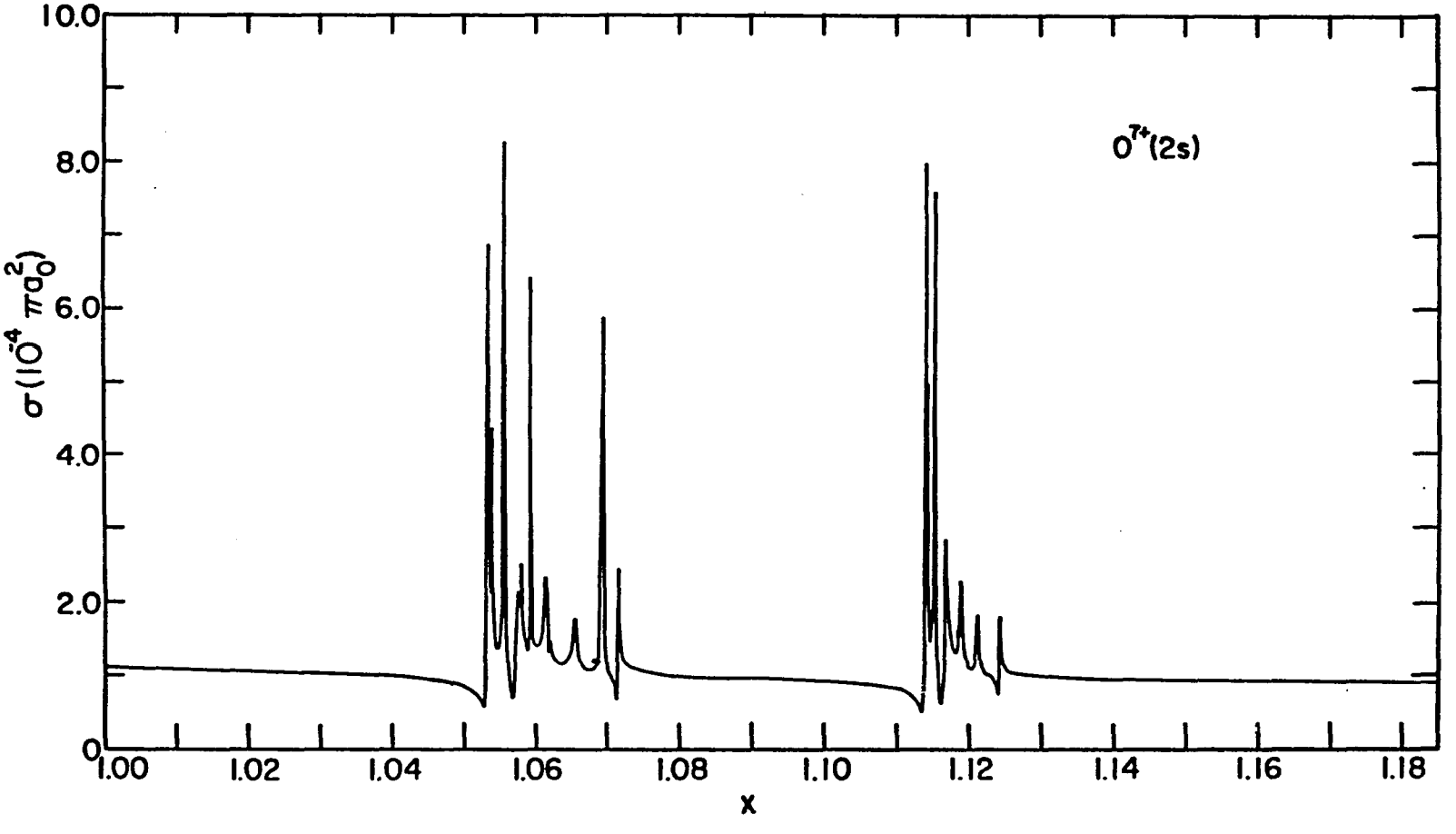
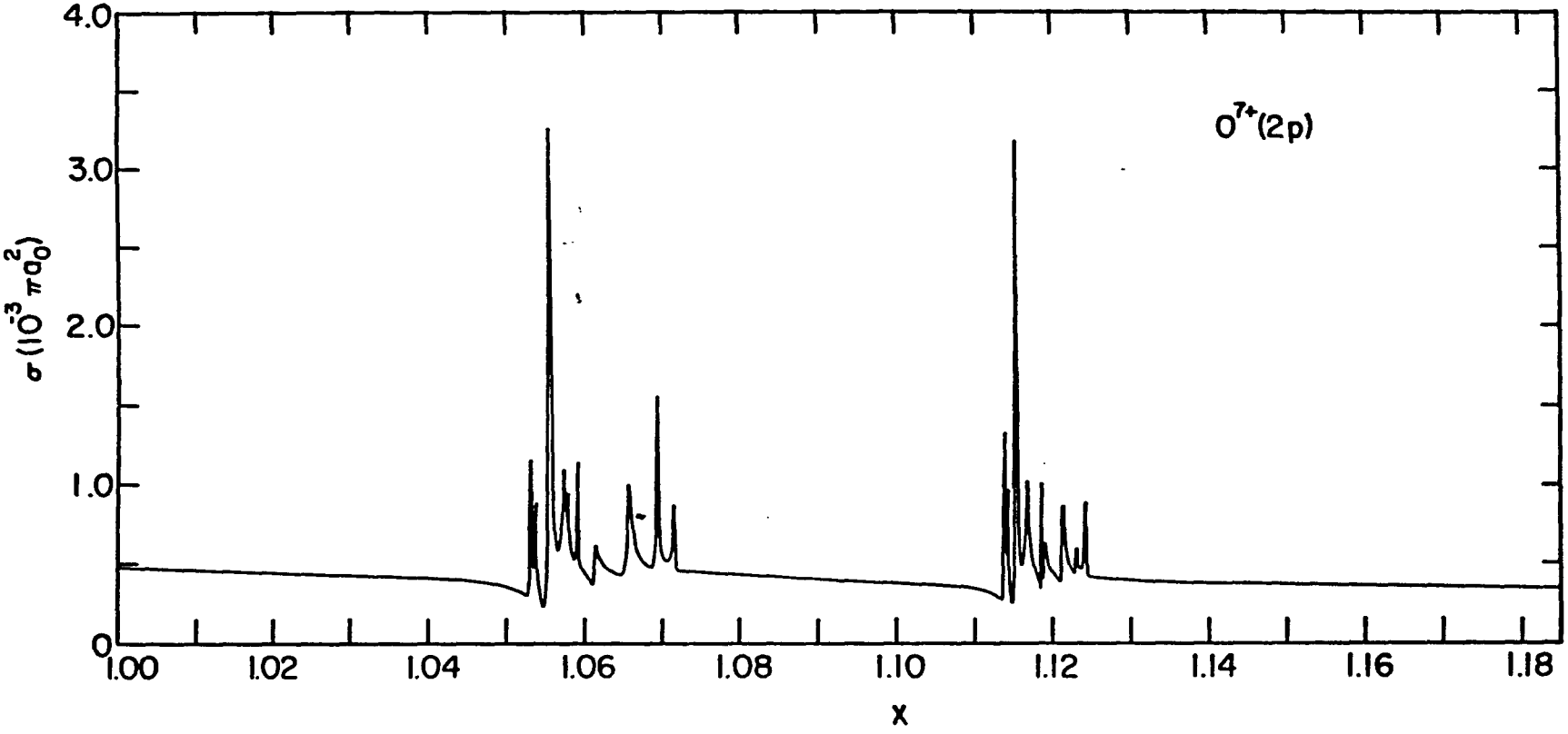
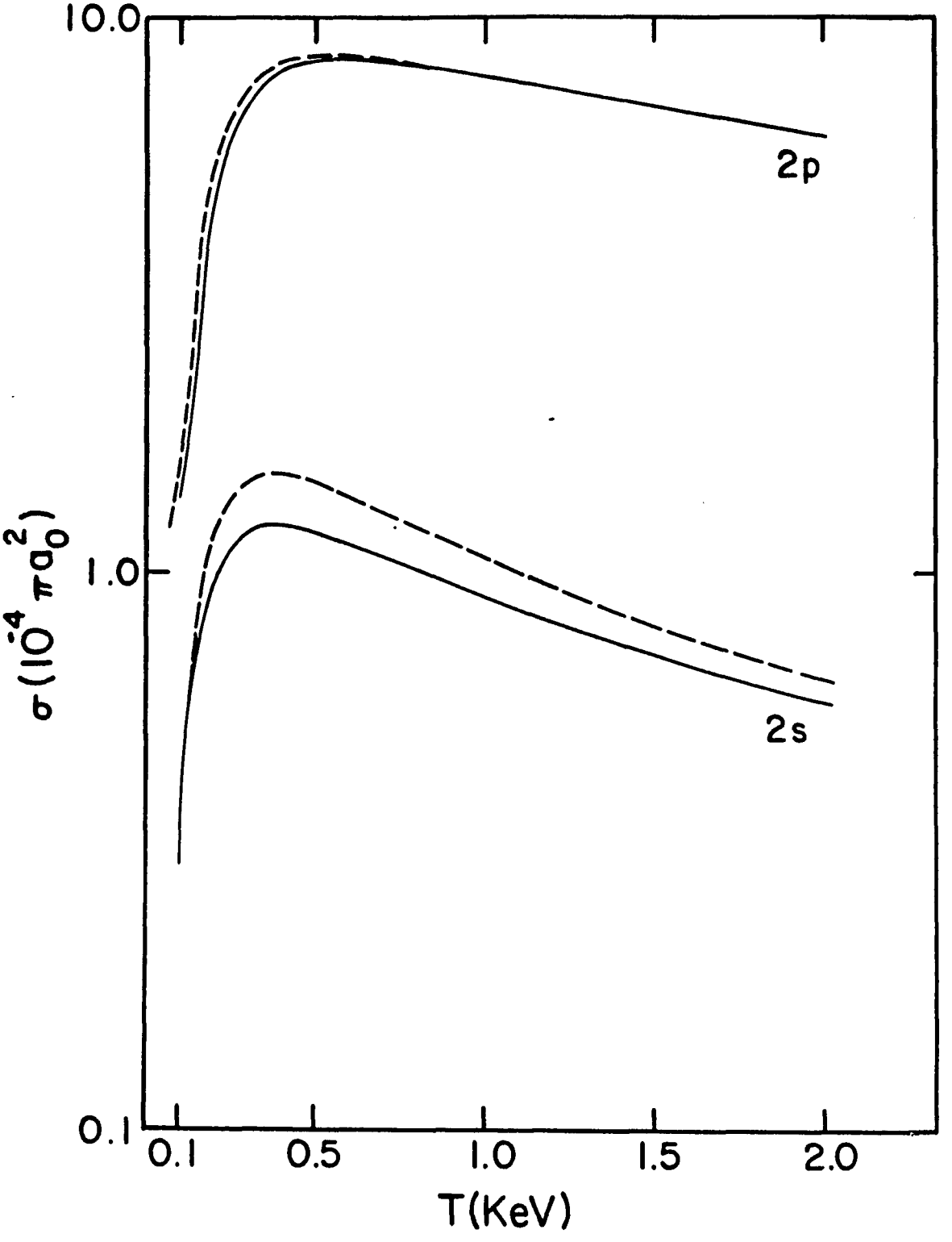
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.00
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
1.18
X

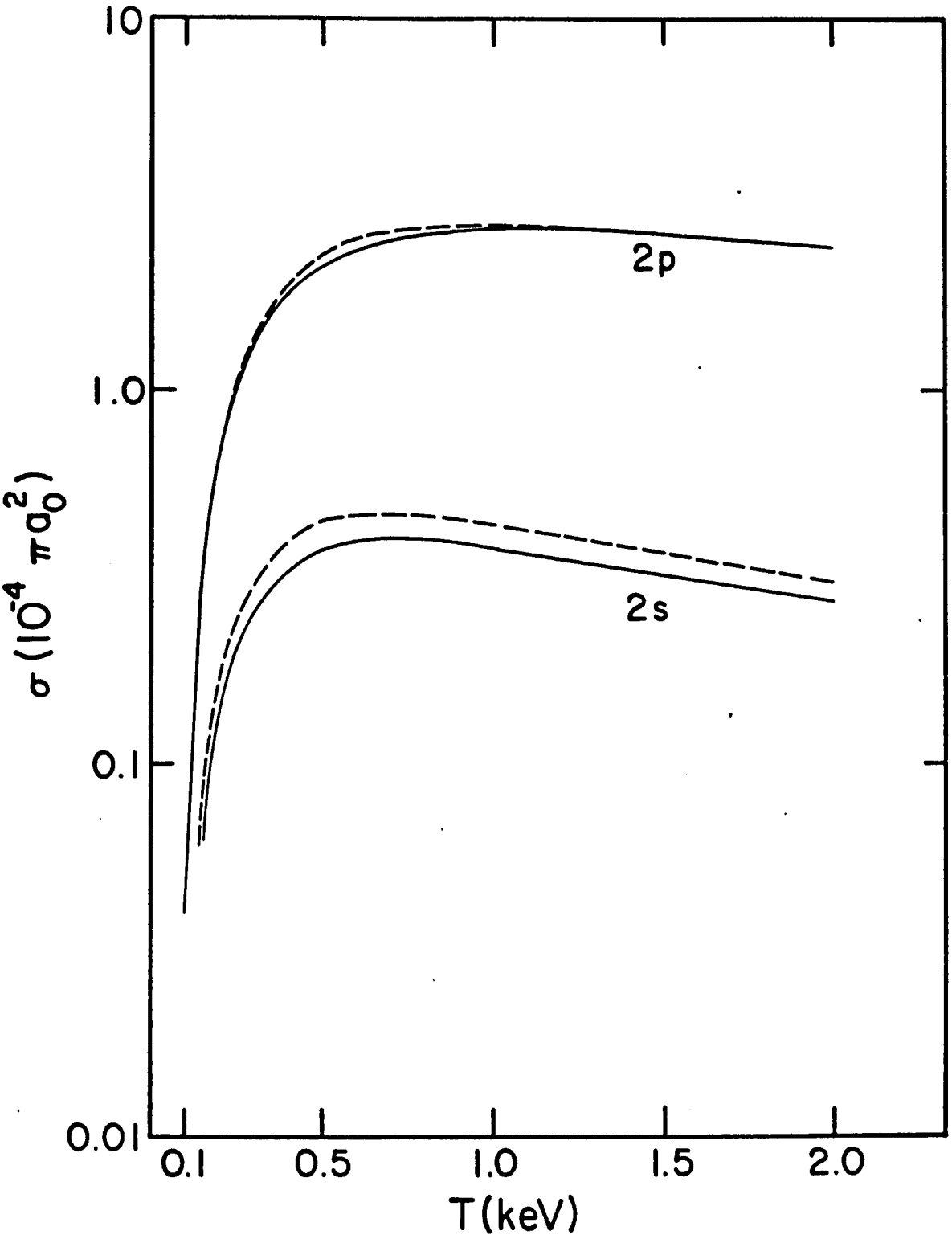

2.0
1.6
1.2
0.8
0.4
0
$\sigma(10^{-3}\pi a_0^2)$
$C^{5+}(2s)$
1.00
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
1.18
x

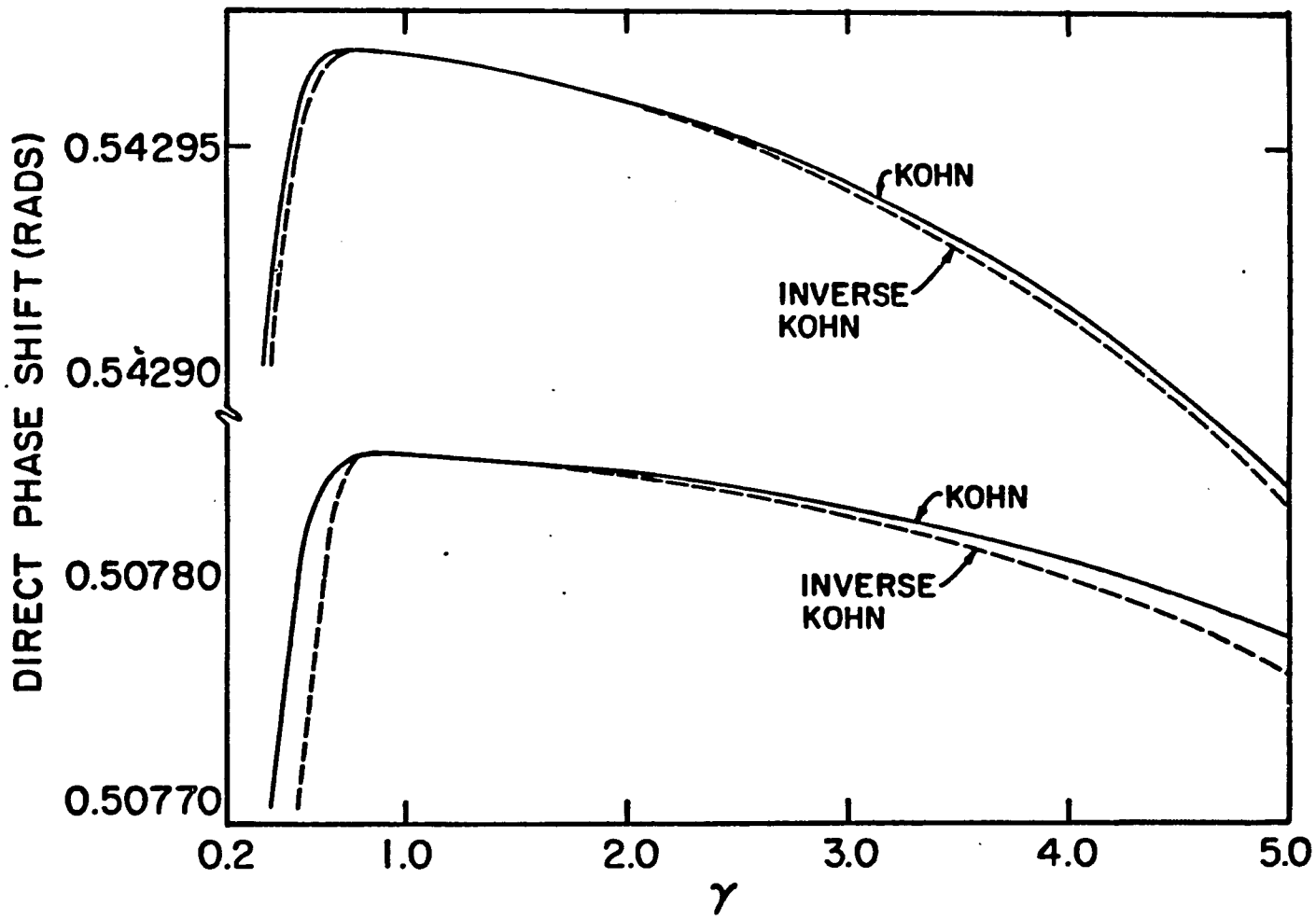

8.0
6.0
4.0
2.0
0
σ(10^-3 πa0^2)
C^5+(2p)
1.00
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
1.18
X

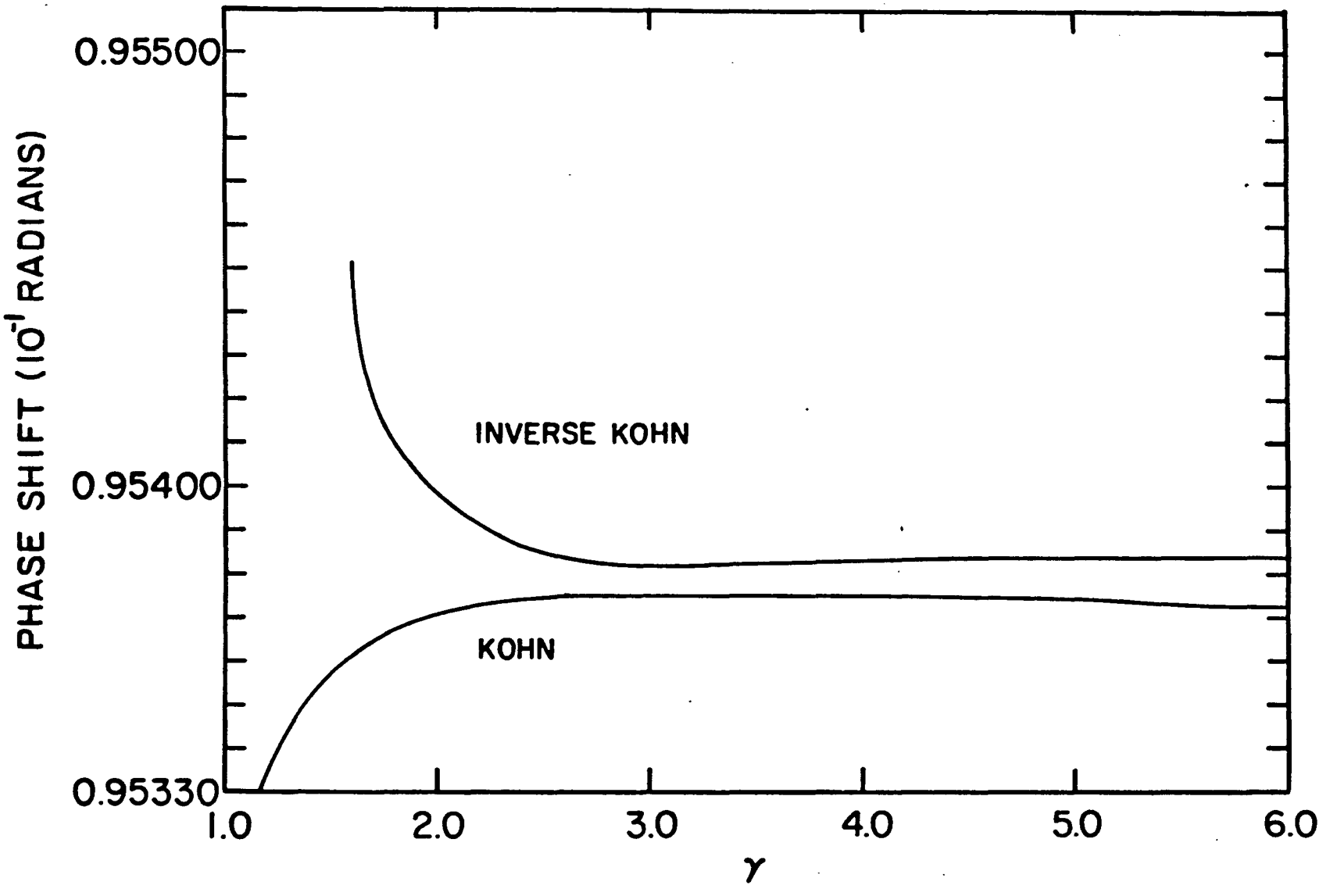

10.0
8.0
6.0
4.0
2.0
0
σ(10^-4 πa_0^2)
0^7+(2s)
1.00
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
1.18
x

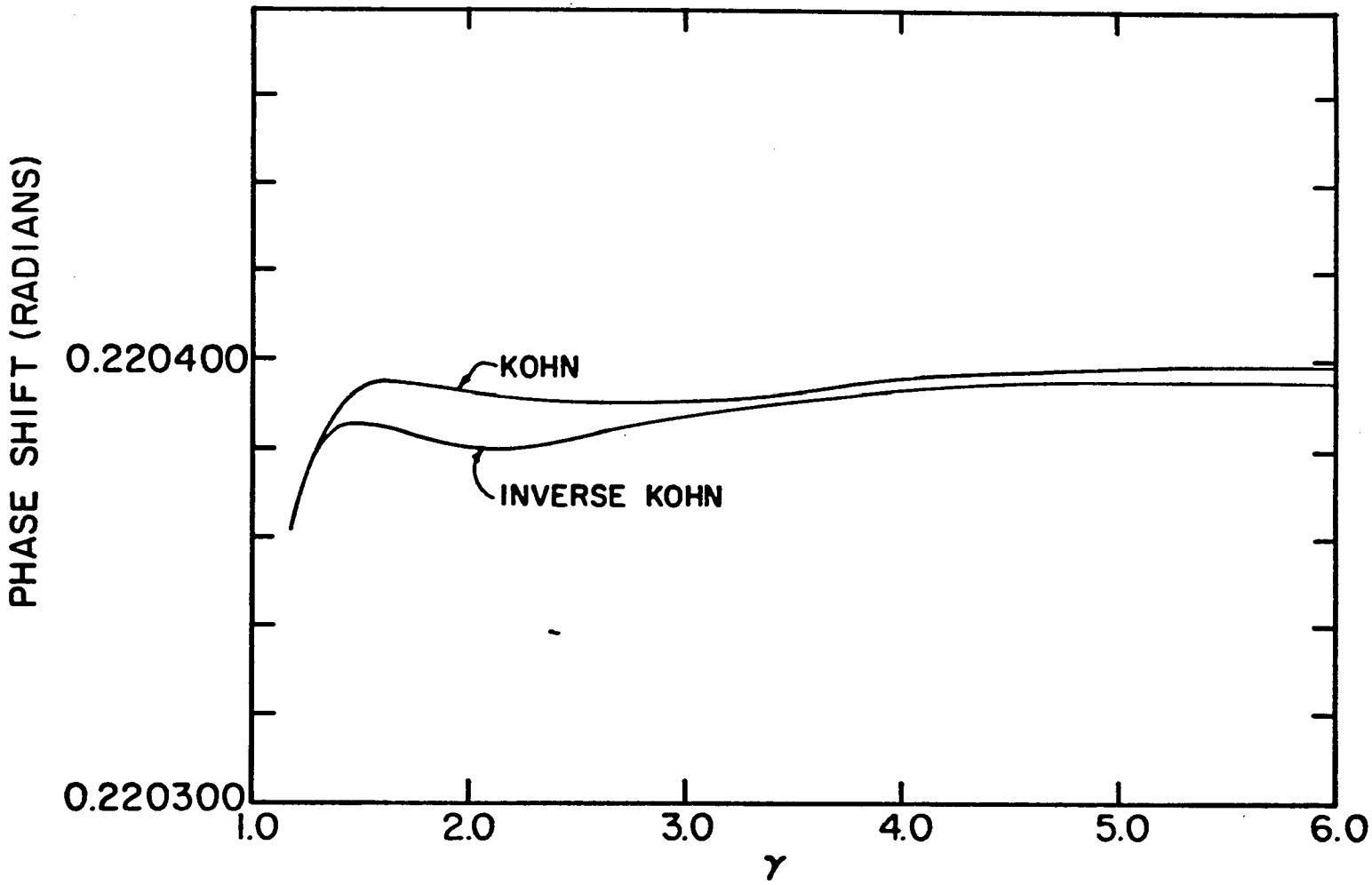

4.0
3.0
2.0
1.0
0
$\sigma(10^{-3}\pi a_0^2)$
$O^{7+}(2p)$
1.00
1.02
1.04
1.06
1.08
1.10
1.12
1.14
1.16
1.18
X

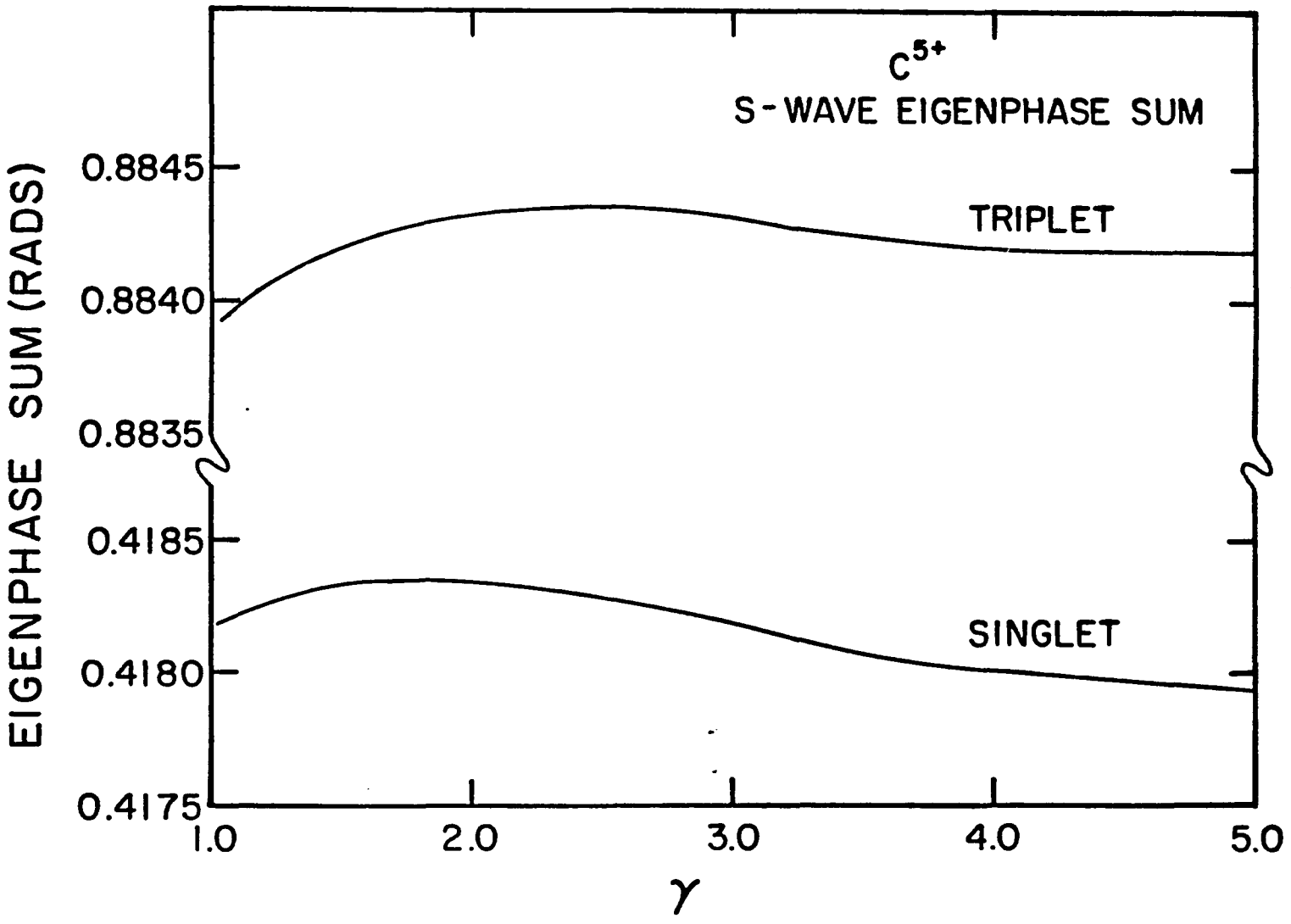

10.0
1.0
0.1
$\sigma(10^{-4}\pi a_0^2)$
2p
2s
0.1
0.5
1.0
1.5
2.0
T(KeV)


10
1.0
0.1
0.01
σ (10⁻⁴ πa₀²)
2p
2s
0.1
0.5
1.0
1.5
2.0
T(keV)


DIRECT PHASE SHIFT (RADS)
0.54295
0.54290
0.50780
0.50770
KOHN
INVERSE KOHN
KOHN
INVERSE KOHN
0.2
1.0
2.0
3.0
4.0
5.0
γ


0.95500
0.95400
0.95330
PHASE SHIFT (10^{-1} RADIANS)
INVERSE KOHN
KOHN
1.0
2.0
3.0
4.0
5.0
6.0
γ


PHASE SHIFT (RADIANS)
0.220400
0.220300
KOHN
INVERSE KOHN
1.0
2.0
3.0
4.0
5.0
6.0
γ


C^{5+}
S-WAVE EIGENPHASE SUM
TRIPLET
SINGLET
EIGENPHASE SUM (RADS)
0.8845
0.8840
0.8835
0.4185
0.4180
0.4175
1.0
2.0
3.0
4.0
5.0
γ

APPENDIX A

OPTIMIZATION OF THE VARIATIONAL PARAMETER γ

This parameter appears in the regularizing factor of the irregular Coulomb function. The dependence of scattering phase shifts on this parameter was considered in two model problems, the scattering of an electron by the static potential

$$U_{00}(r) = -2(Z-1)/r - 2(Z+1/r)e^{-2Zr} \quad . \qquad (A.1)$$

with Z=2 (He^+), and single channel scattering in the static exchange approximation.

Applying the variational method to the first model, we calculated phase shifts at two different energies (k_i^2 = 1.0 Rys. and 2.0 Rys). The parameter γ was varied over the interval (0.2, 5.0) with steps of 0.1. The short range basis for the expansion of the scattering function consisted of 12 Slater orbitals of the type $r^n e^{-Kr}$ where K was fixed at 2.5 and the integer n was varied from 0 to 11. Two expressions, Kohn and Inverse Kohn, of the phase shift (in radians) were compared in Fig. XIX. An optimum of 0.8 was obtained for that case which is independent of energy. The phase shifts show a considerable stability over the interval γ = 0.7 to γ = 4.8, the variation being in the fifth and sixth decimal digits. Such

a stability was also observed when we applied the same method to model two.

The L=0 singlet and triplet phase shifts for scattering of an electron by C^{5+} at an energy of 16.0 Ry, are plotted as a function of the parameter γ in Figs. XX and XXI. Both Kohn and Inverse Kohn values of the phase shifts (singlet and triplet) maintain a stable value as γ varies from 2.4 to 5.6. A suitable value of γ in this case would be 3.6. The short range basis considered in this model consists of 13 Slater orbitals whose exponents ζ_i [see Eq. (2.14)] form a decreasing geometric progression whose ratio is 1.3 and whose maximum element is 15.6. The same procedure has been repeated for He^+ and O^{7+} for which optimum values of γ seemed to scale with the nuclear charge, Z (1.2 for He^+; 4.8 for O^{7+}).

Pushing this discussion further, a more elaborate calculation was done using the 3s-3p set. The stability of the partial L=0 eigenphase sums (singlet and triplet) for scattering by C^{5+} at x = 1.07, is shown very clearly in Fig. XXII. The short range basis used is the one which appears in the first column in Table III.

APPENDIX B

EVALUATION OF THE INTERACTION POTENTIAL RADIAL MATRIX ELEMENTS

These elements are defined by

$$V_\ell^{ij}(r) = \int_0^\infty dx\, x^2 (x^{n_i} e^{-Z_i x}) \frac{x_<}{x_>^{\ell+1}} (x^{n_j} e^{-Z_j x}) \; ;$$

$$(i = 1,\ldots,N_i;\; j = 1,\ldots,N_j) \qquad (B.1)$$

where N_K is the number of elements in the pseudobasis of the K^{th} target state.

In order to evaluate this integral, it is necessary to divide the integration interval as follows

$$V_\ell^{ij}(r) = \int_0^r dx\, x^2 (x^{n_i} e^{-Z_i x}) \frac{x^\ell}{r^{\ell+1}} (x^{n_j} e^{-Z_j x})$$

$$+ \int_r^\infty dx\, x^2 (x^{n_i} e^{-Z_i x}) \frac{r^\ell}{x^{\ell+1}} (x^{n_j} e^{-Z_j x}) \; .$$

This can be rewritten as

$$V_\ell^{ij}(r) = r^{-(\ell+1)} \{ \int_0^\infty dx\, x^{n_i+n_j+\ell+2} e^{-(Z_i+Z_j)x}$$

$$- \int_r^\infty dx\, x^{n_i+n_j+\ell+2} e^{-(Z_i+Z_j)x} \}$$

$$+ r^\ell \int_r^\infty dx\, x^{n_i+n_j+1-\ell} e^{-(Z_i+Z_j)x} \; .$$

Now using analytic expressions of the integrals involved

$$\int_0^\infty dx\ x^n\ e^{-\alpha x} = n!\ \alpha^{-(n+1)}$$

and

$$\int_0^\infty dx\ x^n\ e^{-\alpha x} = \frac{n!}{\alpha^{n+1}}\ e^{-\alpha r} \sum_{p=0}^{n} \frac{(\alpha r)^p}{p!} ,$$

$V_\ell^{ij}(r)$ reduces to

$$V_\ell^{ij}(r) = \frac{(n_i+n_j+\ell+2)!}{(Z_i+Z_j)^{n_i+n_j+\ell+3}\ r^{+1}} \left\{ 1 - e^{-(Z_i+Z_j)x} \sum_{k=0}^{n_i+n_j+\ell+2} \frac{(Z_i+Z_j)^k\ r^k}{k!} \right\}$$

$$+ \frac{(n_i+n_j+1-\ell)!\, r^\ell}{(Z_i+Z_j)^{n_i+n_j+2-\ell}} \cdot e^{-(Z_i+Z_j)r} \sum_{k=0}^{n_i+n_j+1-\ell} \frac{(Z_i+Z_j)^k r^k}{k!} ,$$

which, taking a common factor, is rewritten as

$$V_\ell^{ij}(r) = \frac{(n_i+n_j+\ell+2)!}{(Z_i+Z_j)^{(n_i+n_j+\ell+3)}\, r^{\ell+1}} \left\{ 1 - e^{-(Z_i+Z_j)r} \left[\sum_{k=0}^{n_i+n_j+\ell+2} \frac{(Z_i+Z_j)^k r^k}{k!} - \frac{r^{2\ell+1}(n_i+n_j+1-\ell)!\,(Z_i+Z_j)^{2\ell+1}}{(n_i+n_j+\ell+2)!} \sum_{k=0}^{n_i+n_j+1-\ell} \frac{(Z_i+Z_j)^k r^k}{k!} \right] \right\}$$

The property of the sums which appear above is that the highest two terms cancel out, thus reducing V_ℓ^{ij} to

$$V_\ell^{ij}(r) = \frac{(n_i+n_j+\ell+2)!}{(Z_i+Z_j)^{n_i+n_j+\ell+3}\, r^{\ell+1}} \left\{ 1 - e^{-(Z_i+Z_j)r} \left[\sum_{k=0}^{n_i+n_j+\ell+1} \frac{(Z_i+Z_j)^k r^k}{k!} - \frac{(n_i+n_j+1-\ell)!}{(n_i+n_j+\ell+2)!} \sum_{k=0}^{n_i+n_j-\ell} \frac{(Z_i+Z_j)^{k+2\ell+1}}{k!} r^{k+2\ell+1} \right] \right\}$$

A change of summation index in the second sum

$$k \to \nu - 2\ell - 1 \ ,$$

yields

$$V_\ell^{ij}(r) = \frac{(n_i+n_j+\ell+2)!}{(Z_i+Z_j)^{n_i+n_j+\ell+3} r^{\ell+1}} \left\{ 1 - e^{-(Z_i+Z_j)r} \sum_{\nu=0}^{n_i+n_j+\ell+1} \times h(n_i,n_j;\ell,\nu;Z_i,Z_j) r^\nu \right\} \ , \qquad \text{(B.2)}$$

where h is defined by

$$h = \left[\frac{1}{\nu!} - \frac{(n_i+n_j+1-\ell)!}{(n_i+n_j+\ell+2)!(\nu-2\ell-1)!} \right] (Z_i+Z_j)^\nu \ . \qquad \text{(B.3)}$$

For sufficiently large r, V_ℓ^{ij} reduces to:

$$V_\ell^{ij}(r) \simeq \frac{\alpha_{ij}}{r^{\ell+1}} \ ,$$

where

$$\alpha_{ij} = \frac{(n_i+n_j+\ell+2)!}{(Z_i+Z_j)^{n_i+n_j+\ell+3}} \qquad \text{(B.4)}$$

It is this kind of asymptotic behavior which causes serious oscillations in integrals involving the product of two Coulomb functions and V, these oscillations should be cured in the appropriate manner (Appendix E).

APPENDIX C

EVALUATION OF THE BASIC BOUND-FREE INTEGRAL

$$T_k = \int_0^\infty dr\ r^\lambda e^{-\mu r} (1-e^{-\gamma r})^{j_k}\ U_k(\ell, pr) \qquad (k = 1,2)\ ,$$

(C.1)

Two cases may be distinguished

1) $k = 1$

In this case, U_1 is the regular Coulomb function ($F_\ell(pr)$), hence T_1 may be expressed in terms of the analytic integrals

$$J_\ell(\lambda,\mu) = \int_0^\infty dr\ r^\lambda\ e^{-\mu r}\ F_\ell(pr) \qquad (C.2)$$

In order to accomplish that, the factor $(1-e^{-\gamma r})^{j_k}$ is expanded

$$(1-e^{-\gamma r})^{j_k} = j_k! \sum_{m=0}^{j_k} \frac{(-1)^m e^{-m\gamma r}}{m!\,(j_k-m)!}$$

T_1 then reduces to

$$T_1 = j_k! \sum_{m=0}^{j_k} \frac{(-1)^m}{m!\,(j_k-m)!}\ J_\ell(\lambda, \mu+m\gamma) \qquad (C.3)$$

The problem then reduces to the evaluation of integrals 'J_ℓ'. Again two cases arise

i) $\ell = 0$

Integrals J_o are expressed in terms of the integrals $I_o(\lambda,\mu) = \int_o^\infty dr\ r^\lambda (F_o(pr)/pr) e^{-\mu r}$, which were evaluated in a closed form by Shimamura.[45] We have

$$J_o(\lambda,\mu) = p\ I_o(\lambda+1,\mu) \quad , \quad \lambda \geq -1 \ ; \tag{C.4}$$

where

$$I_o(0,\mu) = \frac{C_o}{2\alpha p} (e^{\alpha\phi}-1) \quad ,$$

$$I_o(1,\mu) = C_o\ e^{\alpha\phi}(\mu^2+p^2)^{-1} \quad ,$$

and

$$I_o(\lambda,\mu) = (\mu^2+p^2)^{-1}[2\{\alpha p+\mu(\lambda-1)\}\ I_o(\lambda-1\ ,\mu)$$

$$- (\lambda-1)(\lambda-2) I_o(\lambda-2\mu)] \quad , \quad \lambda \geq 2 \ ;$$

C_o is the normalization of the Coulomb function for $\ell=0$, α is the Coulomb parameter ($\alpha = -z/p$), and ϕ is defined by

$$\phi = 2 \tan^{-1}(p/\mu) \tag{C.5}$$

(ii) $\ell \geq 1$

In this case, we are looking for recurrence relations which express J_ℓ in terms of lower order integrals ($J_{\ell-1}$, $J_{\ell-2}$,...). To start with, we consider the recurrence relation satisfied by the Coulomb function[46]

$$\left\{(\ell+1)^2+\alpha^2\right\}^{1/2} F_{\ell+1}(\rho) = \left\{\frac{(\ell+1)^2}{\rho} + \alpha\right\} F_\ell(\rho) - (\ell+1)\frac{dF_\ell}{d\rho}\,, \tag{C.6}$$

where $\rho = pr$, and then operate with $\int_0^\infty dr\, r^\lambda\, e^{-\mu r}$. Equation (C.6) reduces to

$$\left\{(\ell+1)^2+\alpha^2\right\}^{1/2} J_{\ell+1}(\lambda,\mu) = \frac{(\ell+1)^2}{p} J_\ell(\lambda-1,\mu) + \alpha\, J_\ell(\lambda,\mu) - \frac{(\ell+1)}{p}\int_0^\infty r^\lambda\, e^{-\mu r}\frac{dF_\ell}{dr} \tag{C.7}$$

The integral which appears in Eq. (C.7) is evaluated by parts

$$\int_0^\infty dr\, r^\lambda\, e^{-\mu r}\frac{dF_\ell}{dr} = \mu\, J_\ell(\lambda,\mu) - \lambda J_\ell(\lambda-1,\mu) + \left[r^\lambda\, e^{-\mu r}\, F_\ell(pr)\right]_0^\infty \tag{C.8}$$

The last equation can be further reduced by considering the following

$$\lim_{r\to\infty} [r^{\lambda}\, e^{-\mu r}\, F_{\ell}(pr)] = 0 \ ,$$

and

$$\lim_{r\to 0} [r^{\lambda}\, e^{-\mu r}\, F_{\ell}(pr)] = \lim_{r\to 0} r^{\lambda}\, \varepsilon_{\ell}(pr) \ ;$$

where ε_{ℓ} is the near-zero behavior of the regular Coulomb function

$$\varepsilon_{\ell}(pr) = (pr)^{\ell+1}\, C_{\ell}(\alpha) \ .$$

Eq. (C.8) becomes

$$\lim_{r\to 0} [r^{\lambda}\, e^{-\mu r}\, F_{\ell}(pr)] = p^{\ell+1}\, C_{\ell}(\alpha) \lim_{r\to 0} r^{\lambda+\ell+1} \ ,$$

which diverges for "$\lambda \leq -\ell-2$"; otherwise

$$\lim_{r\to 0} r^{\lambda}\, \varepsilon_{\ell}(pr) = \begin{cases} 0 & , \quad \lambda \geq -\ \ell \\ C_{\ell}(\alpha) p^{\ell+1} & , \quad \lambda = -\ell-1 \end{cases} \qquad \text{(C.9)}$$

Now combining Eqs. (C.9) and (C.8), the recurrence relation (C.7) splits into

$$P(\ell^2+\alpha^2)^{1/2}\, J_\ell(\lambda,\mu) = \begin{cases} {}^{\ell}p^{\ell}C_{\ell-1}+(\alpha p-\mu\ell)J_{\ell-1}(\lambda,\mu) & , \lambda = -\ell \\ \ell(\lambda+\ell)J_{\ell-1}(\lambda-1,\mu)+(\alpha p-\mu\ell)J_{\ell-1}(\lambda,\mu), & \\ \qquad\qquad \lambda \geq 1-\ell & \end{cases}$$

(C.10)

One case remains to investigate: $\lambda = -\ell-1$. In order to establish a recurrence relation for this particular integral, we consider the Coulomb differential equation

$$\left[\frac{d^2}{dr^2} + p^2 - 2\alpha p/r - \frac{\ell(\ell+1)}{r^2} \right] F_\ell(pr) = 0 ,$$

and operate with "$\int_0^\infty dr\, r^{\lambda+2}\, e^{-\mu r}$". This yields

$$J''_\ell(\lambda+2,\mu) + p^2 J_\ell(\lambda+2,\mu) - 2\alpha p J_\ell(\lambda+1,\mu) - \ell(\ell+1)J_\ell(\lambda,\mu) = 0$$

(C.11)

Integrating J''_ℓ by parts gives

$$J''(\lambda+2,\mu) = \int_0^\infty dr\ r^{\lambda+2}\ e^{-\mu r}\ \frac{d^2F_\ell(pr)}{dr^2}$$

$$= \mu J'_\ell(\lambda+2,\mu) - (\lambda+2)J'_\ell(\lambda+1,\mu)$$

$$+ [r^{\lambda+2}\ e^{-\mu r}\ F'_\ell(pr)]_0^\infty \ .$$

The last term vanishes for large $r(r\to\infty)$. For small r, we have[47]

$$F'_\ell(\rho) = C_\ell(\rho)\rho^\ell\ [(\ell+1) + \frac{\alpha(\ell+2)}{\ell+1}\ \rho] + O(r^{\ell+2}) \ .$$

Then

$$\lim_{r\to 0} r^{\lambda+2}\ e^{-\mu r}\ F'_\ell(pr) = p^\ell(\ell+1)C_\ell(\alpha) \lim_{r\to 0} r^{\lambda+\ell+2}$$

which vanishes for our case $(\lambda=-\ell-1)$. Equation (C.11) reduces to:

$$J''_\ell(\lambda+2,\mu) = \mu J'_\ell(\lambda+2,\mu) - (\lambda+2)J'_\ell(\lambda+1,\mu) \qquad \text{(C.12)}$$

Repeating the same procedure for J'_ℓ, we get the relation

$$J'_\ell(\lambda+2,\mu) = \mu J_\ell(\lambda+2,\mu) - (\lambda+2)J_\ell(\lambda+1,\mu) \ ,$$

which, when combined with Eq. (C.12), yields

$$J''_{\ell}(\lambda+2,\mu) = \mu^2 J_{\ell}(\lambda+2,\mu) - 2\mu(\lambda+2)J_{\ell}(\lambda+1,\mu)$$

$$+ (\lambda+1)(\lambda+2)J_{\ell}(\lambda,\mu) \ .$$

Substituting in Eq. (C.11) gives

$$(\mu^2+p^2)J_{\ell}(\lambda+2,\mu) - 2[\alpha p+\mu(\lambda+2)]\ J_{\ell}(\lambda+1,\mu)$$

$$+ [(\lambda+1)(\lambda+2) - \ell(\ell+1)]\ J_{\ell}(\lambda,\mu) = 0 \qquad \text{(C.13)}$$

which is an extension of the recurrence relation given by Shimamura[45] for "$\ell=0$".

Rearranging terms in Eq. (C.13) and substituting "$\lambda = -\ell-1$", we get

$$J_{\ell}(-\ell-1,\mu) = \frac{1}{2\ell} \left\{ (\mu^2+p^2)J_{\ell}(1-\ell,\mu) \cdot \right.$$

$$\left. - 2[\alpha p-\mu(\ell-1)]\ J_{\ell}(-\ell,\mu) \right\}, \qquad \text{(C.14)}$$

which can be expressed in terms of lower order integrals by using the recurrence relations (C.10) already established. Equation (C.11) thus becomes

$$J_{\ell}(-\ell-1,\mu) = \frac{(\ell^2+\alpha^2)^{-1/2}}{2p\ell} \left\{ [\ell(\mu^2+p^2) - 2(\alpha p-\mu\ell)(\alpha p-\mu\ell+\mu)] \right.$$

$$J_{\ell-1}(-\ell,\mu) + (\mu^2+p^2)(\alpha p-\mu\ell)J_{\ell-1}(1-\ell,\mu)$$

$$- 2\ell p^{\ell} C_{\ell-1}(\alpha)\,(\alpha p - \mu\ell + \mu)\Big\} \quad .$$

In order to simplify notations, we define

$$A_\ell = [p(\ell^2+\alpha^2)^{1/2}]^{-1} \quad ,$$

$$B_\ell = (\alpha p - \mu\ell) \quad ,$$

and

$$E = (\mu^2+p^2) \quad .$$

The recurrence relations then reduce to:

$$\begin{cases} J_\ell(-\ell-1,\mu) = \dfrac{A_\ell}{2\ell}\Big\{[\ell E - 2B_{\ell-1}B_\ell]J_{\ell-1}(-\ell,\mu) \\ \qquad\qquad + B_\ell E\, J_{\ell-1}(1-\ell,\mu) - 2\ell p^{\ell} C_{\ell-1}B_{\ell-1}\Big\} \\ J_\ell(-\ell,\mu) = A_\ell\Big\{B_\ell J_{\ell-1}(-\ell,\mu) + \ell p^{\ell}\, C_{\ell-1}\Big\} \\ J_\ell(\lambda,\mu) = A_\ell\Big\{\ell(\lambda+\ell)J_{\ell-1}(\lambda-1,\mu) + B_\ell J_{\ell-1}(\lambda,\mu)\Big\} \quad , \quad \lambda \geq 1-\ell \end{cases} \tag{C.15}$$

Still, in the case "$\lambda \leq -\ell-2$" the T integral is evaluated numerically. Actually, the integral $J_\ell(\lambda,\mu)$ diverges for $\lambda < (-\ell-1)$.

2) $k = 2$

The case "$\ell=0$" has also been treated in the same reference.[45] The author evaluated the integral

$$I_1(\lambda,\mu) = \int_0^\infty dr\ r^\lambda \frac{G_o(pr)}{pr} e^{-\mu r} \qquad (\lambda \geq 0)$$

Defining the angular variable ϕ as in (C.5), he expressed these integrals in terms of the function $f_\alpha(\phi)$. (α is the Coulomb parameter)

$$\begin{cases} I_1(0,\mu) = -f_\alpha(\phi)/C_o p \\ I_1(1,\mu) = [\mu-2\alpha p f_\alpha(\phi)]/C_o p(\mu^2+p^2) \\ I_1(2,\mu) = [2(\mu+\alpha p)C_o p\ I_1(1,\mu)-1]/C_o p(\mu^2+p^2) \\ I_1(\lambda,\mu) = (\mu^2+p^2)^{-1}\ \{2[\alpha p+\mu(\lambda-1)]\ I_1(\lambda-1,\mu) \\ \qquad - (\lambda-1)(\lambda-2)\ I_1(\lambda-2,\mu)\}\ ,\ \lambda \geq 3\ . \end{cases}$$

The function $f_\alpha(\phi)$ satisfies the differential equation

$$\frac{df_\alpha(\phi)}{d\phi} = \alpha\, f_\alpha(\phi) - \frac{1}{2}\cot\frac{\phi}{2} \quad , \qquad \phi\varepsilon[0,2\pi] \; ;$$

whose solution is written as

$$f_\alpha(\phi) = e^{-\alpha(\pi-\phi)} \left[B_\alpha + \frac{1}{2}\int_0^{\pi-\phi} dt\, e^{\alpha t} \tan\frac{t}{2}\right]$$

where

$$B_\alpha = f_\alpha(\pi) = \sum_{n=1}^{\infty} \frac{(-1)^n n}{n^2+\;^2} \quad .$$

This constant B_α was expressed as a finite sum and a correction term which was approximated by an integral

$$B_\alpha \simeq \sum_{m=1}^{M} \frac{\alpha^2-2m(2m-1)}{[\alpha^2+(2m)^2][\alpha^2+2m-1)^2]} + \frac{1}{4}\,\ell n\left[1 - \frac{4M+1}{\alpha^2+(2M+1)^2}\right]$$

However, we found that this approach was impractical to use. The difficulty is that the integral which appears in the solution of $f_\alpha(\phi)$ diverges for most cases of interest in which ϕ approaches the limits of the segment $[0,2\pi]$. Such a case is

$$p << 1 \quad \text{with} \quad \mu \quad \text{finite} \quad ,$$

which is typical of the 2s and 2p channels at low incident energies. Shimamura pointed out that such divergences

occur but are eliminated by the fact that only differences of such functions are calculated

$$I_1(\lambda,\mu) - I_1(\lambda,\mu') \quad ;$$

despite this, numerical difficulties are still very probable except possibly at energies (not approaching zero) below the n=2 threshold, where we have used these integrals successfully. Otherwise, integrals of the type T_2 are evaluated numerically.

APPENDIX D

EXPANSION OF COULOMB FUNCTIONS IN THE ASYMPTOTIC REGION

We use the notations of C. E. Fröberg,[47] to express the regular and irregular Coulomb functions as an expansion for large ρ

$$\begin{cases} F_L = f \sin \theta_L + g \cos \theta_L \\ G_L = f \cos \theta_L - g \sin \theta_L \ , \end{cases} \qquad (D.1)$$

where

$$\theta_L(\rho) = \rho - \eta \ \ell n \ 2\rho - L \ \pi/2 + \sigma_L \quad (\rho = pr) \ , \qquad (D.2)$$

$$f \sim \Sigma \ f_k \ ,$$

and

$$g \sim \Sigma \ g_k \ .$$

The quantities f_k and g_k satisfy the recurrence relations

$$\begin{cases} f_{k+1} = a_k f_k - b_k g_k \ , \quad f_o = 1 \ ; \\ g_{k+1} = a_k g_k + b_k f_k \ , \quad g_o = 0 \ ; \end{cases} \qquad (D.3)$$

where

$$a_k = \frac{(2k+1)\eta}{s(k+1)\rho} \quad ,$$

and

$$b_k = \frac{L(L+1)+\eta^2-k(k+1)}{2(k+1)\rho} \tag{D.4}$$

For convenience, we define

$$A_k = r\, a_k \quad ,$$

and

$$B_k = r\, b_k \tag{D.5}$$

and keep only terms with r^{-3} dependence; that is

$$f \simeq f_0 + f_1 + f_2 + f_3 \quad ,$$

and

$$g \simeq g_0 + g_1 + g_2 + g_3 \quad ;$$

which combining Eqs. (D.3), (D.4) and (D.5) can be written as

$$f \simeq 1 + \frac{A_0}{r} + \frac{A_1A_0-B_1B_0}{r^2} + \frac{A_2(A_1A_0-B_1B_0)-B_2(A_1B_0+B_1A_0)}{r^3}$$

and

$$g \simeq \frac{B_0}{r} + \frac{A_1B_0+B_1A_0}{r^2} + \frac{A_2(A_1B_0+B_1A_0)+B_2(A_1A_0-B_1B_0)}{r^3}$$

These expressions may now be written in a compact form by redefining the constants, that is

$$f \simeq 1 + \frac{A}{r} + \frac{C}{r^2} + \frac{E}{r^3}$$

$$g \simeq \frac{B}{r} + \frac{D}{r^2} + \frac{F}{r^3} \qquad \text{(D.6)}$$

The Coulomb phase which appears in Eq. (D.2), is determined as follows

i) For $L = 0$, σ_0 is given by[46,48]

$$\sigma_0 = -\eta\, C_e + \sum_{s=1}^{\infty} (\eta/s - \tan^{-1} \eta/s) \ ,$$

C_e being the Eulers constant (0.5772156649...).

In practice, the sum is carried out up to some large number N, and the remainder is replaced by integral over s; that is

$$\sum_{s=1}^{\infty} (\eta/s - \tan^{-1} \eta/s) \simeq \sum_{s=1}^{N} (\eta/s - \tan^{-1} \eta/s)$$

$$+ \sum_{N+1}^{\infty} [\eta/s - (\eta/s - \tfrac{1}{3}\, \eta^3/s^3)]$$

Replacing $\sum_{N+1}^{\infty} s^{-3}$ by $\int_{N+1}^{\infty} ds\, s^{-3}$, we get

$$\sigma_0 = -\eta\, C_e + \sum_{s=1}^{N} (\eta/s - \tan^{-1} \eta/s) + \frac{\eta^3}{6(N+1)^2} \quad .$$

ii) For $L > 0$, we use the recurrence relation

$$\sigma_L = \sigma_0 + \sum_{s=1}^{L} \tan^{-1} (\eta/s)$$

APPENDIX E

EVALUATION OF THE INTEGRALS

$$J_{ij}(\lambda) = \int_R^\infty \frac{dr}{r^{\lambda+1}} U_i^A(\ell_p, pr) U_j^A(\ell_q, qr) \; ; \; \lambda = 1,2,... \tag{E.1}$$

(U_k^A is an asymptotic Coulomb function).

In order to evaluate these integrals; that is, we consider

$$F_{\ell p}(pr) = f^p \sin \theta_{\ell p} + g^p \cos \theta_{\ell p}$$

$$G_{\ell p}(pr) = f^p \cos \theta_{\ell p} - g^p \sin \theta_{\ell p}$$

and

$$F_{\ell q}(qr) = f^q \sin \theta_{\ell q} + g^q \cos \theta_{\ell q}$$

$$G_{\ell q}(qr) = f^q \cos \theta_{\ell q} - g^q \sin \theta_{\ell q} \; ,$$

and form the different products

$$F_{\ell p}F_{\ell q} = f^p f^q \sin\theta_{\ell p} \sin\theta_{\ell q} + f^p g^q \sin\theta_{\ell p} \cos\theta_{\ell q}$$

$$+ f^p g^q \sin\theta_{\ell q} \cos\theta_{\ell p} + g^p g^q \cos\theta_{\ell p} \cos\theta_{\ell q}$$

$$F_{\ell p}G_{\ell q} = f^p f^q \sin\theta_{\ell p} \cos\theta_{\ell q} - f^p g^q \sin\theta_{\ell p} \sin\theta_{\ell q}$$

$$+ f^q g^p \cos\theta_{\ell p} \cos\theta_{\ell q} - g^p g^q \cos\theta_{\ell p} \sin\theta_{\ell q}$$

$$F_{\ell q}G_{\ell p} = f^p f^q \cos\theta_{\ell p} \sin\theta_{\ell q} + f^p g^q \cos\theta_{\ell p} \cos\theta_{\ell q}$$

$$- g^p f^q \sin\theta_{\ell p} \sin\theta_{\ell q} - g^p g^q \sin\theta_{\ell p} \cos\theta_{\ell q}$$

$$G_{\ell p}G_{\ell q} = f^p f^q \cos\theta_{\ell p} \cos\theta_{\ell q} - fpg^p \cos\theta_{\ell p} \sin\theta_{\ell q}$$

$$- f^q g^p \sin\theta_{\ell p} \cos\theta_{\ell q} + g^p g^q \sin\theta_{\ell p} \sin\theta_{\ell q}$$

The products of f's and g's are evaluated using Eqs. (D.6), and retaining terms up to the order of r^{-3} only

$$f^p f^q \simeq 1 + \frac{A^p + A^q}{r} + \frac{C^p + C^q + A^p A^q}{r^2} + \frac{E^p + E^q + A^p C^q + A^q C^p}{r^3}$$

$$f^p g^q \simeq \frac{B^q}{r} + \frac{D^q + A^p B^q}{r^2} + \frac{F^q + A^p D^q + C^p B^q}{r^3}$$

$$f^q g^p \simeq \frac{B^p}{r} + \frac{D^p + A^q B^p}{r^2} + \frac{F^p + A^q D^p + C^q B^p}{r^3}$$

$$g^p g^q \simeq \frac{B^p B^q}{r^2} + \frac{B^p D^q + B^q D^p}{r^3} \quad .$$

By appropriately redefining the coefficients, these expressions may be written as

$$f^p f^q \simeq \sum_{k=1}^{3} A_k / r^k \qquad f^q g^p \simeq \sum_{k=1}^{3} C_k / r^k$$

$$f^p g^q \simeq \sum_{k=1}^{3} B_k / r^k \qquad g^p g^q \simeq \sum_{k=1}^{3} D_k / r^k \qquad \text{(E.3)}$$

knowing that

$$A_0 = 1 \quad , \quad \text{and} \quad B_0 = C_0 = D_0 = D_1 = 0 \quad .$$

Combining Eqs. (E.3), (E.2) and (E.1), the integrals $J_{ij}(\lambda)$ are expressed as

$$J_{00}(\lambda) \simeq \sum_{k=1}^{3} \{A_k K_{00}(\lambda+k) + B_k K_{01}(\lambda+k) + C_k K_{10}(\lambda+k)$$

$$+ D_k K_{11}(\lambda+k)\}$$

$$J_{01}(\lambda) \simeq \sum_{k=1}^{3} A_k K_{01}(\lambda+k) - B_k K_{00}(\lambda+k) + C_k K_{11}(\lambda+k)$$

$$- D_k K_{10}(\lambda+k)\}$$

$$J_{10}(\lambda) \simeq \sum_{k=1}^{3} A_k K_{10}(\lambda+k) + B_k K_{11}(\lambda+k) - C_k K_{00}(\lambda+k)$$

$$- D_k K_{01}(\lambda+k)\}$$

$$J_{11}(\lambda) \simeq \sum_{k=1}^{3} A_k K_{11}(\lambda+k) - B_k K_{10}(\lambda+k) - C_k K_{01}(\lambda+k)$$

$$+ D_k K_{00}(\lambda+k)\} \quad ; \qquad \text{(E.4)}$$

where

$$K_{ij}(\lambda) \equiv \int_R^\infty \frac{dr}{r^{\lambda+1}} \zeta_i(\ell_p, pr)\zeta_j(\ell_p, pr) \quad ; \qquad \text{(E.5)}$$

with

$$\zeta_0(\ell, kr) \equiv \sin \theta_{\ell_k}(kr)$$

and

$$\zeta_1(\ell,kr) \equiv \cos\ \theta_{\ell_k}(kr) \ .$$

From Eq. (D.2), the angles are given by

$$\theta_{\ell_p}(pr) = pr - \eta_p\ \ell n\ 2pr - \ell_p\ \pi/2 + \sigma_{\ell_p}$$

$$\theta_{\ell_q}(qr) = qr - \eta_q\ \ell n\ 2qr - \ell_q\ \pi/2 + \sigma_{\ell_q} \ . \qquad \text{(E.6)}$$

In order to evaluate these integrals, we introduce the following trigonometric relations

$$\sin\theta_{\ell_p}\ \sin\theta_{\ell_q} = \tfrac{1}{2}\ [\cos(\theta_{\ell_p}-\theta_{\ell_q}) - \cos(\theta_{\ell_p}+\theta_{\ell_q})]$$

$$\sin\theta_{\ell_p}\ \cos\theta_{\ell_q} = \tfrac{1}{2}\ [\sin(\theta_{\ell_p}+\theta_{\ell_q}) + \sin(\theta_{\ell_p}-\theta_{\ell_q})]$$

$$\cos\theta_{\ell_p}\ \sin\theta_{\ell_q} = \tfrac{1}{2}\ [\sin(\theta_{\ell_p}+\theta_{\ell_q}) - \sin(\theta_{\ell_p}-\theta_{\ell_q})]$$

$$\cos\theta_{\ell_p}\ \cos\theta_{\ell_q} = \tfrac{1}{2}\ [\cos(\theta_{\ell_p}-\theta_{\ell_q}) + \cos(\theta_{\ell_p}+\theta_{\ell_q})] \ ;$$

which, using the relation

$$e^{i\theta} = \cos\theta + i\sin\theta \quad ,$$

may be rewritten as

$$\sin\theta_{\ell_p}\sin\theta_{\ell_q} = \tfrac{1}{2}\,\mathrm{Re}[e^{i\delta}-e^{i\sigma}]$$

$$\sin\theta_{\ell_p}\cos\theta_{\ell_q} = \tfrac{1}{2}\,\mathrm{Im}[e^{i\delta}+e^{i\sigma}]$$

$$\cos\theta_{\ell_p}\sin\theta_{\ell_q} = \tfrac{1}{2}\,\mathrm{Im}[e^{i\delta}-e^{i\sigma}]$$

$$\cos\theta_{\ell_p}\cos\theta_{\ell_q} = \tfrac{1}{2}\,\mathrm{Re}[e^{i\delta}+e^{i\sigma}] \quad , \qquad \text{(E.7)}$$

where

$$\delta = \theta_{\ell_p} - \theta_{\ell_q} \quad ,$$

and

$$\sigma = \theta_{\ell_p} + \theta_{\ell_q} \quad .$$

Using Eq. (E.6), we express δ and σ as

$$\delta = (p-q)r + \ell n\, r^{-(\eta_p-\eta_q)} - \eta_p \ell n 2p + \eta_q \ell n 2q - (\ell_p-\ell_q)\pi/2 + \sigma_{\ell_p} - \sigma_{\ell_q}$$

$$\sigma = (p+q)r + \ell n\, r^{-(\eta_p+\eta_q)} - \eta_p \ell n 2p - \eta_q \ell n 2q - (\ell_p+\ell_q)\pi/2 + \sigma_{\ell_p} + \sigma_{\ell_q} \; ;$$

Hence

$$e^{i\sigma} = \Sigma_o \, r^{-i(\eta_p+\eta_q)} \, e^{i(p+q)r}$$

$$e^{i\delta} = \Delta_o \, r^{-i(\eta_p-\eta_q)} \, e^{i(p-q)r} \quad , \tag{E.8}$$

where

$$\Sigma_o = \exp i[\sigma_{\ell_p}+\sigma_{\ell_q}-\eta_p \ell n 2p-\eta_q \ell n 2q-(\ell_p+\ell_q)\pi/2]$$

$$\Delta_o = \exp i\,[\sigma_{\ell_p}-\sigma_{\ell_q}-\eta_p \ell n 2p+\eta_q \ell n 2q-(\ell_p-\ell_q)\pi/21 \quad .$$

(E.9)

Now combining Eqs. (E.7), (E.8), (E.9), and (E.5), the integrals can be expressed in the form

$$K_{00}(\lambda) = -\,\mathrm{Re}(\Delta) \qquad K_{10}(\lambda) = \mathrm{Im}(\Delta)$$

$$K_{01}(\lambda) = \mathrm{Im}(\Sigma) \qquad K_{11}(\lambda) = \mathrm{Re}(\Sigma) \quad , \tag{E.10}$$

in which

$$\Sigma = \tfrac{1}{2}\,[\Sigma_o \cdot \varepsilon(\lambda,p+q,\eta_p+\eta_q) + \Delta_o \cdot \varepsilon(\lambda,p-q,\eta_p-\eta_q)]$$

$$\Delta = \tfrac{1}{2}\,[\Sigma_o \cdot \varepsilon(\lambda,p+q,\eta_p+\eta_q) - \Delta_o \cdot \varepsilon(\lambda,p-q,\eta_p-\eta_q)] \quad . \tag{E.11}$$

The function "ε" just introduced, is an exponential type integral defined by

$$\varepsilon(\lambda,a,b) = \int_R^\infty \frac{dr}{r^{\lambda+1}}\, r^{-ib}\, e^{iar} \quad , \tag{E.12}$$

which is integrated by parts until it converges. It may explicitly be written as

$$\varepsilon(\lambda,a,b) = \frac{ie^{i(aR-b\ell nR)}}{aR^{\lambda+1}} \left\{ 1 + \sum_{n=1}^{N} \frac{\left[\prod_{m=1}^{n} (\lambda+m+ib) \right]}{(iaR)^n} \right\}$$

$$+ \text{ correction term} \tag{E.13}$$

The summation is carried to an integer "N", large enough for the correction term to become negligible. A special case arises when

$$a = b = 0 \quad \text{and} \quad \lambda \geq 1 \; ; \quad \text{then}$$

$$\varepsilon(\lambda,0,0) = \frac{1}{\lambda R^\lambda} \quad . \tag{E.14}$$

Other special cases of interest are

i) $p = q = K$ and $\ell_p = \ell_q = \ell$

which is typical of an $(n\ell\text{-}n\ell)$ transition; for example, a 2p-2p transition. In this case, the expressions for

Σ_o and Δ_o, simplify to

$$\Sigma_o^* = (-1)^{\ell} \exp 2i(\sigma_\ell - \eta_k \ell n\ 2k)$$

$$\Delta_o^* = 1$$

and the expressions for Σ and Δ reduce to

$$\Sigma = \frac{1}{2} [\Sigma_o \cdot \varepsilon(\lambda, 2k, 2\eta_k) + (\lambda R^{\lambda})^{-1}]$$

$$\Delta = \frac{1}{2} [\Sigma_o\ \varepsilon(\lambda, 2k, 2\eta_k) - (\lambda R^{\lambda})^{-1}] \quad .$$

ii) $p = q = k$ and $\ell_p = \ell_q + 1$

which is typical of an ($n\ell$-$n\ell$+1) transition, for example a 2s-2p transition. Again Equation (E.9) reduces to

$$\Sigma_o = i(-1)^{\ell+1} \exp i[2\sigma_\ell + \tan^{-1} \frac{\eta}{\ell+1} - 2\eta_k\ \ell n\ 2k\ ]$$

$$\Delta_o = -i \exp i[\tan^{-1} \frac{\eta}{\ell+1}\ ] \quad ,$$

where we use $\ell = \ell_q$ and

$$\sigma_{\ell_p} = \sigma_{\ell_q} + \tan^{-1} \frac{\eta}{\ell_q+1}$$

iii) $p \neq q$ and $\ell_p = \ell_q + 1$

which is typical of an $(n\ell\text{-}n'\ell{+}1)$ transition, like a 1s-2p transition. In this case, the expressions for Σ_o and Δ_o are reduced by using

$$\ell = \ell_q$$

and

$$\sigma_{\ell_p} = \sigma_{\ell_q} + \tan^{-1} \frac{\eta}{\ell_q + 1} \quad .$$

APPENDIX F

NUMERICAL INTEGRATION SCHEME

The formula used is an 11-point Newton-Cote formula[46] of the closed type, which approximates the function (integrand) by a tenth order polynomial. In each interval

$$\int_{x_0}^{x_{10}} f(x)dx = \frac{5h}{299376}\{16067(f_0+f_{10}) + 106300(f_1+f_9)$$

$$- 48525(f_2+f_8) + 272400(f_3+f_7)$$

$$- 260550(f_4+f_6) + 427368\ f_5\}$$

$$- \frac{1346350}{326918592}\ f^{(12)}(\xi)k^{13} \quad ,$$

where h is the mesh size and

$$f_n = f(x_0 + nh) \quad .$$

This method is powerful in the sense that the mesh size could be large, thus the number of points is considerably decreased. The error is of the order of h^{13}.

PROGRAMS/SUBPROGRAMS

```
      FUNCTION AITCH(M,N,LP,NU,A,Z)
C*****************************************************************
C     WRITTEN BY DR J. CALLAWAY
C     COMPUTES COEFFICIENTS OCCURRING IN INTEGRAL OF TWO SLATER ORBITALS
C     TIMES (RLESS**LP/RGREAT**LP+1)
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      ANU=NU+1
      GNU=DGAMMA(ANU)
      SPQ=0.0
      NUL=NU-2*LP
      IF(NUL.LE.0)GO TO 1
      AMN=M+N+2-LP
      GMN=DGAMMA(AMN)
      ABC=M+N+3+LP
      GBC=DGAMMA(ABC)
      ANUL=NUL
      GNL=DGAMMA(ANUL)
      SPQ=GMN/(GNL*GBC)
    1 X=1./GNU-SPQ
      AZ=1.
      IF(NU.EQ.0)GO TO 2
      AZ=(A+Z)**NU
    2 AITCH=AZ*X
      RETURN
      END
```

```
      DOUBLE PRECISION FUNCTION ANGL(LEM,LA,LB,LC,LD,LL1)
C*********************************************************************
C     WRITTEN BY DR J. CALLAWAY
C     COMPUTES THE ANGULAR FACTOR
C     LAMBDA=LEM . LA,LB,LC & LD ARE THE INDIVIDUAL ANGULAR MOMENTA ,
C     LL1 IS THE TOTAL ANGULAR MOMENTUM
C     C3J IS THE 3J SYMBOL
C*********************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      C3J(L,M,N)=DSQRT(
     1      FACTR(L+N-M)*FACTR(L-M+N)*FACTR(-L+M+N)/FACTR(L+M+N+1)*(FACTR
     2 ((L+M+N)/2)/(FACTR((L+M-N)/2)*FACTR((L-M+N)/2)*FACTR((-L+M+N)/2)
     3 ))**2)*(-1.)**((L+M+N)/2)
      ANGL=0.D0
      L12=(LA+LC+LEM)/2
      R13=(LA+LC+LEM)/2.D0
      R12=L12
      IF(R12.NE.R13) GO TO 5
      L12=(LB+LD+LEM)/2
      R13=(LB+LD+LEM)/2.D0
      R12=L12
      IF(R12.NE.R13) GO TO 5
      CT=F6J(2*LA,2*LB,2*LL1,2*LD,2*LC,2*LEM)
      IF(CT.EQ. 0.D0) GO TO 5
      DT=(2.*LA+1.)*(2.*LB+1.)*(2.*LC+1.)*(2.*LD+1.)
      ANGL=(-1.)**(LA+LC-LL1)*C3J(LA,LC,LEM)*C3J(LD,LD,LEM)*DSQRT(DT)*CT
  5   RETURN
      END
```

```
      FUNCTION BBDIR(KB,B,M,Z,L,J,C,N,A)
C*****************************************************************************
C     WRITTEN BY Dr J. CALLAWAY
C     COMPUTES MATRIX ELEMENT OF RLESS**L/RGREAT**L+1 BETWEEN SLATER
C     ORBITALS R2**KB*EXP(-BR2) R2**J*EXP(-CR2) R1**M EXP(-ZR1)
C     R1**N*EXP(-AR1) (R1*R2)**2
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      MN3=M+N+L+3
      AMN=MN3
      BMN=DGAMMA(AMN)
      AZ=A+Z
      BC=B+C
      AZBC=AZ+BC
      KJ2=KB+J+2-L
      AKJ=KJ2
      BKJ=DGAMMA(AKJ)
      DS=BKJ/(BC**KJ2)
      MX=MN3-1
      DO 3 IA=1,MX
      NU=IA-1
      KJN=KJ2+NU
      IF(IA.GT.1)GO TO 1
      CK=BKJ
      GO TO 2
    1 Q=KJN-1
      CK=CK*Q
    2 DS=DS-AITCH(M,N,L,NU,A,Z)*CK/(AZBC**KJN)
    3 CONTINUE
      BBDIR=DS*BMN/(AZ**MN3)
      RETURN
      END
```

```
      SUBROUTINE DINT(J,F,DR,Y)
C*****************************************************************************
C     ESTIMATES THE INTEGRAL OF F(I)  (I=1,J)  USING THE 11-POINT NEWTON-
C     COTE CLOSED TYPE FORMULA (WITH CONSTANT MESH SIZE DR) AND THE
C     TRAPEZOIDAL RULE FOR TAIL POINTS.
C     THE OUTPUT(Y) HAS AN ERROR OF THE ORDER OF DR**13
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION F(J)
      Y=0.0
      II=1
      IF(J.EQ.1)  RETURN
      IF(J.EQ.2) GO TO 10
      IN=(J-1)/10+1
      IF(IN.EQ.1.AND.J.LT.11) GO TO 10
      DO 5 K=1,IN
      IJ=II+10
      IF(K.EQ.IN.AND.(J-II+1).LT.11) GO TO 10
      YMULT=5.D0*DR/299376.D0
      Z=YMULT*(160867.D0*(F(II)+F(IJ))+106300.D0*(F(II+1)+F(IJ-1))-48525.
     1D0*(F(II+2)+F(IJ-2))+272400.D0*(F(II+3)+F(IJ-3))-260550.D0*(F(II+4
     2)+F(IJ-4))+427363.D0*F(II+5))
      Y=Z+Y
    5 II=IJ
      RETURN
   10 IF((J-II+1).EQ.1) RETURN
      Y=Y+0.5D0*DR*(F(II)+F(J))
      IF((J-II+1).EQ.2.OR.J.EQ.2)  RETURN
      I1=II+1
      J1=J-1
      DO 15 L=I1,J1
   15 Y=Y+DR*F(L)
      RETURN
      END
```

```
      FUNCTION CBFKE(II,J2,L2,B2,P,NAT,A,LA,LP,NB,B,NZT,ZT,LQ,LZ,E,Z)
C*****************************************************************
C     COMPUTES RADIAL SINGLE-ELECTRON-HAMILTONIAN CONTRIBUTION TO
C     EXCHANGE BOUND-FREE MATRIX ELEMENTS
C     THE INTEGRAL IS EVALUATED NUMERICALLY FOR II=1 (THE INTEGRAND
C     IN THAT CASE INVOLVES THE IRREGULAR COULOMB FUNCTION)
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200),F(1200)
      COMMON/BFR/FF(1200),GF(1200)
      COMMON/RODE/DR,R,NM
      DAB=DFLOAT(NAT+NB+1)
      AB=A+B
      F1=DFACTR(NAT+NB)/AB**(NAT+NB+3)
      B1=F1*DAB*(DAB+1.D0)
      A1=-(B**2+E)
      A2=2.D0*(B*DFLOAT(NB+1)-Z)
      A3=DFLOAT(LQ*(LQ+1)-NB*(NB+1))
      C1=-ZT**2
      C2=2.D0*(ZT*DFLOAT(NZT+1)-Z)
      C3=DFLOAT(LP*(LP+1)-NZT*(NZT+1))
      F1=F1*(A1*(DAB+1.D0)*DAB+A2*AB*DAB+A3*AB**2)
      IF(II.EQ.1) GO TO 1
      CBFKE=(B1*C1+F1)*CTIB(II,NZT+2-L2,J2,ZT,B2,P,LP,FP,GP,    Z)+C2*B1*
     1CTIB(II,NZT+1-L2,J2,ZT,B2,P,LP,FP,GP,Z)
      IF(LP.EQ.NZT.OR.NZT.EQ.(-LP-1)) RETURN
      CBFKE=CBFKE+B1*C3*CTIB(II,NZT-L2,J2,ZT,B2,P,LP,FP,GP,Z)
      RETURN
    1 DO 2 I=1,NM
      X=R(I)
      V=X**(NZT-L2)*DEXP(-ZT*X)*((B1*C1+F1)*X**2+B1*C2*X
     1  +B1*C3)
      IF(J2.NE.0) V=V*(1.D0-DEXP(-B2*X))**J2
    2 F(I)=V*GF(I)
      CALL DQDB11(NM,DR,F,YY)
      CBFKE=YY
      RETURN
      END
```

```
      FUNCTION CBFFIN(II,KB,J2,L2,LP,B,BETA,P,Z)
C*****************************************************************
C     COMPUTES RADIAL KINETIC ENERGY CONTRIBUTION TO DIRECT BOUND-FREE
C     MATRIX ELEMENTS.THE INTEGRAL IS EVALUATED NUMERICALLY WHEN II=1,
C     THE INTEGRAND CONTAINS THEN THE IRREGULAR COULOMB FUNCTION
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200),F(1200)
      COMMON/NODE/DR,R,NM
      COMMON/BFR/FP(1200),GP(1200)
      IF(J2.EQ.0.AND.L2.EQ.1) GO TO 10
      A1=-(B**2+P**2)
      A2=2.D0*(B*DFLOAT(KB+1)-Z)
      A3=DFLOAT(LP*(LP+1)-KB*(KB+1))
      IF(II.EQ.1)GO TO 1
      CBFKIN=A1*CTIB(II,KB+2-L2,J2,B,BETA,P,LP,FP,GP,   Z)+A2*CTIB(II,KB
     1+1-L2,J2,B,BETA,P,LP,FP,GP,Z)
      IF(KB.EQ.LP.OR.KB.EQ.(-LP-1))  RETURN
      CBFKIN=CBFKIN+A3*CTIB(II,KB-L2,J2,B,BETA,P,LP,FP,GP,Z)
      RETURN
    1 DO 2 I=1,NM
      X=R(I)
      V=X**(KB-L2)*(A1*X**2+A2*X+A3)*DEXP(-B*X)
      IF(J2.NE.0)V=V*(1.D0-DEXP(-BETA*X))**J2
    2 F(I)=V*GP(I)
      CALL DQDB11(NM,DR,F,YY)
      CBFKIN=YY
      RETURN
   10 CBFKIN=-2.D0*CTIB(II,KB-L2+1,J2,B,BETA,P,LP,FP,GP,Z)
      RETURN
      END
```

```
      SUBROUTINE CBFMX(BFD,BFX,SD,SX)
C*****************************************************************************
C     COMPUTES DIRECT (BFD) AND EXCHANGE (BFX) BOUND-FREE INTEGRALS :
C     MATRIX ELEMENTS OF (H-E) BETWEEN SLATER ORBITALS AND ONE REGULARIZED
C     COULOMB FUNCTION.H IS THE TOTAL HAMILTONIAN . E IS THE TOTAL ENERGY.
C     REQUIRES : CBFXCH,CBFKIN,CTIB,CBFKE
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION BFD(10,2),BFX(10,2)
      DIMENSION SD(10,10),SX(10,10)
      DIMENSION  CEIG(5,10,10),NPWR(5,10),Z(5,10) ,ENEG(5,10)
      DIMENSION R(1200)
      COMMON/BFR/FPC(1200),GPC(1200)
      COMMON/BODE/DELR,R,NPTS
      COMMON/ADC/GAM,E,CEIG,Z,       P,Q,B,C,ENEG,L,LZ,LQ,LA,LP,NBSA,NBSZ
     1,NPWR,L2,L1,KB,JC,NA,NZ,NMAX,NZCH
      ZCH=DFLOAT(NZCH)
      KL=KB+1-L2
      JZ=LZ+1
      JA=LA+1
      DO 40 IIA=1,2
      II=IIA-1
      IF(II.EQ.0) J2=L2-1
      IF(II.EQ.1) J2=2*LP+L2
      DO 15 I=1,NBSZ
      NZT=NPWR(JZ,I)
      TZ=Z(JZ,I)
      DO 15 J=1,NBSA
      DKX=0.0
      DPD=0.0
      DPX=0.0
      DCA=DABS(CEIG(JA,NA,J))
      IF(DCA.LT.1.0D-10)GO TO 14
      NAT=NPWR(JA,J)
      TA=Z(JA,J)
      IF(LP.EQ.LZ.AND.LA.EQ.LQ) DKX=CBFKE(II,J2,L2,GAM,P,NAT,TA,LA,LP,KB
     1,B,NZT,TZ,LQ,LZ,E,ZCH)
      LLX=LA+LZ
      LLQ=LA+LQ
      LLP=LP+LZ
      LLY=LQ+LP
      LMX=MAX0(LLQ,LLX,LLY,LLP)+1
      DO 10 LL=1,LMX
      LM=LL-1
      QQ=ANGL(LM,LZ,LQ,LA,LP,L)
      QN=DABS(QQ)
      IF(QN.LT.1.0D-08)GO TO 5
      DPD=DPD+QQ*CBFXCH(II,P,L2,GAM,J2,KB,B,LM,TZ,NZT,NAT,TA,ZCH,LP)
    5 QR=ANGL( LM,LQ,LZ,LA,LP,L)
      QX=DABS(QR)
      IF(QX.LT.1.0D-08)GO TO 10
      DPX=DPX+QR*CBFXCH(II,P,L2,GAM,J2,NZT,TZ,LM,B,KB,NAT,TA,ZCH,LP)
   10 CONTINUE
   14 SD(I,J)=2.D0*DPD
   15 SX(I,J)=DKX+2.D0*DPX
      DO 35 I=1,NBSZ
      DS=0.0
      DX=0.0
      IF(LP.EQ.LQ.AND.LA.EQ.L2.AND.I.EQ.NA) DS=CBFKIN(II,KB,J2,L2,LP,B,
     1GAM,P,ZCH)
```

```
      DO 31 MA=1,MBSA
      DCA=DABS(CEIG(JA,MA,MA))
      IF(DCA.LT.1.0D-10)GO TO 31
      DO 30 MZ=1,MBSZ
      DS=DS+CEIG(JZ,I,MZ)*SD(MZ,MA)*CEIG(JA,MA,MA)
      DX=DX+CEIG(JZ,I,MZ)*SX(MZ,MA)*CEIG(JA,MA,MA)
   30 CONTINUE
   31 CONTINUE
      BFD(I,IIA)=DS
   35 BFX(I,IIA)=DX
   40 CONTINUE
      RETURN
      END
```

```
      FUNCTION CBFXCH(II,P,L2,B2,J2,N,ZT,L,D,KD,M,A,Z,LP)
C*****************************************************************
C     COMPUTES RADIAL 2-ELECTRON POTENTIAL (P<**L/R>**(L+1)) CONTRIBUT
C     -ION TO DIRECT AND EXCHANGE BOUND-FREE INTEGRALS.THE INTEGRAL IS
C     EVALUATED NUMERICALLY FOR II=1 (THE INTEGRAND WOULD THEN CONTAIN
C     THE IRREGULAR COULOMB FUNCTION)
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200),F(1200)
      COMMON/BFR/FPC(1200),GPC(1200)
      COMMON/BODE/DR,R,NM
      IF(II.EQ.1)GO TO 2
      LIM=N+KD+L+2
      AB=A+B
      SUM=0.D0
      DO 1 NU=1,LIM
      IN=NU-1
    1 SUM=SUM+AITCH(KB,N,L,IN,A,B)*CTIB(II,N+IN+1-L-L2,J2,ZT+AB,B2,P,LP,
     *FPC,GPC,Z)
      Y=CTIB(II,N+1-L-L2,J2,ZT,B2,P,LP,FPC,GPC,Z)-SUM
      CBFXCH=Y*DFACTR(LIM)/AB**(LIM+1)
      RETURN
    2 DO 3 I=1,NM
      X=R(I)
      V=X**(N+2-L2)*DEXP(-ZT*X)*XK12(N,A,KB,D,L,X)
      IF(J2.NE.0)V=V*(1.D0-DEXP(-B2*X))**J2
    3 F(I)=V*GPC(I)
      CALL DQB11(NM,DR,F,YY)
      CBFXCH=YY
      RETURN
      END
```

```
      SUBROUTINE CBMAT(BND,BNX,SD,SX)
C*****************************************************************
C     COMPUTES DIRECT (BND) AND EXCHANGE (BNX) BOUND-BOUND INTEGRALS :
C     MATRIX ELEMENTS OF (H-E) BETWEEN SLATER ORBITALS.
C     H IS THE TOTAL HAMILTONIAN. E IS THE TOTAL ENERGY.
C     REQUIRES : CBXKE,BBDIR,FACTR
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION ENEG(5,10)
      DIMENSION  CEIG(5,10,10),NPWR(5,10),Z(5,10)
      DIMENSION SD(10,10),SX(10,10)
      DIMENSION BND(10,10),BNX(10,10)
      COMMON/ARC/GAM,E,CEIG,Z,      P,Q,B,C,ENEG,L,LZ,LQ,LA,LP,NBSA,NBSZ
     1,NPWR,L2,L1,KB,JC,NA,NZ,NMAX,NZCH
      ZCH=DFLOAT(NZCH)
      JZ=LZ+1
      JA=LA+1
      DO 15 I=1,NBSZ
      NZT=NPWR(JZ,I)
      TZ=Z(JZ,I)
      DO 15 J=1,NBSA
      NAT=NPWR(JA,J)
      TA=Z(JA,J)
      DKX=0.0
      DPD=0.0
      DPX=0.0
      IF(LP.EQ.LZ.AND.LA.EQ.LQ) DKX=CBXKE(TZ,B,NZT,KB,LZ,LQ,TA,C,NAT,JC,
     1LA,LP,E,ZCH)
      LLX=LA+LZ
      LLQ=LA+LQ
      LLP=LP+LZ
      LLY=LQ+LP
      LMX=MAX0(LLQ,LLX,LLY,LLP)+1
      DO 10 LL=1,LMX
      LM=LL-1
      QQ=ANGL(LM,LZ,LQ,LA,LP,L)
      QN=DABS(QQ)
      IF(QN.LT.1.0D-08) GO TO 5
      DPD=DPD+QQ*BBDIR(KB,B,NZT,TZ,LM,JC,C,NAT,TA)
    5 QR=ANGL( LM,LQ,LZ,LA,LP,L)
      QX=DABS(QR)
      IF(QX.LT.1.0D-08)GO TO 10
      DPX=DPX+QR*BBDIR(NZT,TZ,KB,B,LM,JC,C,NAT,TA)
   10 CONTINUE
      SD(I,J)=2.D0*DPD
   15 SX(I,J)=DKX+2.D0*DPX
      DO 35 I=1,NBSZ
      DO 35 J=1,NBSA
      DS=0.0
      DX=0.0
      IF(LP.EQ.LQ.AND.LA.EQ.LZ.AND.I.EQ.J)GO TO 20
      GO TO 25
   20 KJ=KB+JC+1
      P2P=E-ENEG(JA,J)
      BC=B+C
      AKJ=DFLOAT(KJ)
      BKJ=FACTR(KJ-1)
      JJ=JC*(JC+1)
      AJ=DFLOAT(LP*(LP+1)-JJ)
```

```
      DS=BKJ*(AL+2.D0*AKJ*(C*AJ-ZCH )/BC-AKJ*(AKJ+1.D0)*(C*C+P2P)/(BC**2
     1))/(BC**RJ)
   25 DO 31 MZ=1,MRSZ
      DCZ=DABS(CEIG(JZ,I,MZ))
      IF(DCZ.LT.1.0D-10)GO TO 31
      DO 30 MA=1,MRSA
      DCA=DABS(CEIG(JA,J,MA))
      IF(DCA.LT.1.0D-10)GO TO 30
      DS=DS+CEIG(JZ,I,MZ)*SD(MZ,MA)*CEIG(JA,J,MA)
      DX=DX+CEIG(JZ,I,MZ)*SX(MZ,MA)*CEIG(JA,J,MA)
   30 CONTINUE
   31 CONTINUE
      BND(I,J)=DS
   35 BNX(I,J)=DX
      RETURN
      END
```

```
      FUNCTION CBXKE(ZT,B,NZT,NB,LZ,LQ,A,C,NAT,NC,LA,LP,E,Z)
C*****************************************************************************
C     COMPUTES THE RADIAL SINGLE PARTICLE HAMILTONIAN CONTRIBUTION
C     TO EXCHANGE BOUND-BOUND INTEGRALS
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      A1=-(E+A**2)
      A2=2.D0*(A*DFLOAT(NAT+1)-Z)
      A3=DFLOAT(LA*(LA+1)-NAT*(NAT+1))
      C1=-C**2
      C2=2.D0*(C*DFLOAT(NC+1)-Z)
      C3=DFLOAT(LP*(LP+1)-NC*(NC+1))
      AB=A+B
      ZC=ZT+C
      N3=-(NZT+NC+3)
      N3=-(NAT+NB+3)
      D1=DFLOAT(NAT+NB+1)
      D2=D1+1.D0
      E1=DFLOAT(NZT+NC+1)
      E2=E1+1.D0
      CBXKE=DFACTR(NZT+NC)*DFACTR(NAT+NB)*ZC**N3*AB**N3*(D2*D1*E2*E1*(A1
     1+C1)+D1*E1*(E2*A2*AB+D2*C2*ZC)+E2*E1*A3*AB**2+D2*D1*C3*ZC**2)
      RETURN
      END
```

```
      FUNCTION CDIR(II,P,L2,B2,J2,N,ZT,L,IJ,Q,L1,B1,J1,M,A,LP,LQ,Z)
C*****************************************************************
C     COMPUTES 2-ELCTRON RADIAL POTENTIAL CONTRIBUTION TO DIRECT FPFE
C     -FREE MATRIX ELEMENTS.FOR VALUES OF THE VARIABLE L GT. 0
C     THE INTEGARL IS EVALUATED NUMERICALLY UP TO SOME R-MAX THEN
C     CORRECTED BY AN ANALYTIC TERM (THE REASON IS THE OSCILLATORY
C     NATURE OF THE INTEGRAND)
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200),P(1200)
      COMMON/BORE/DELR,R,NM
      COMMON/FPFE/FP(1200),GP(1200),DFP(1200),DGP(1200),FQ(1200),GQ(1200)
      LM=L+L1+L2-2
      LAM=N+M+L+3
      APC=DFACTR(LAM-1)/((A+ZT)**LAM)
      NP=NM
      RMXM=R(NP)
      DO 10 I=1,NP
      RHO=R(I)
      B1R=-B1*RHO
      B2R=-B2*RHO
      XK=XK12(M,ZT,N,A,L,RHO)
      IF(L.EQ.0)XK=XK-APC/RHO
      V=RHO**(2-L1-L2)*XK
      IF(J1.NE.0)  V=V*(1.D0-DEXP(B1R))**J1
      IF(J2.NE.0)  V=V*(1.D0-DEXP( B2P))**J2
      IF(II.EQ.1)  GO TO 7
      IF(IJ.EQ.1)  GO TO 4
      P(I)=V*FP(I)*FQ(I)
      GO TO 10
    4 P(I)=V*FP(I)*GQ(I)
      GO TO 10
    7 IF(IJ.EQ.1)  GO TO 8
      P(I)=V*GP(I)*FQ(I)
      GO TO 10
    8 P(I)=GP(I)*GQ(I)*V
   10 CONTINUE
      CALL DQB11(NP,DELR,P,Y)
      CDIR=Y
      IF(L.EQ.0)RETURN
      CDIR=CDIR+APC*CORINT(II,IJ,LP,LQ,P,Q,LM,Z,RMXM)
      END
```

```
      FUNCTION CEKIB(IJ,II,J1,J2,L1,L2,LP,B,Q,P)
C*****************************************************************
C     COMPUTES RADIAL KINETIC ENERGY CONTRIBUTION TO DIRECT FREE-FREE
C     MATRIX ELEMENTS
C     THE INTEGRAL IS EVALUATED NUMERICALLY FOR ALL COMBINATIONS OF
C     II & IJ=0,1
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200),F(1200)
      COMMON/BODE/DELR,R,NM
      COMMON/FPR/FP(1200),GP(1200),DFP(1200),DGP(1200),FQ(1200),GQ(1200)
      IF(L2.EQ.1.AND.J2.EQ.0)GO TO 9
      DL2=DFLOAT(L2)
      DJ2=DFLOAT(J2)
      DO 10 I=1,NM
      BR=-B*R(I)
      DBR=DEXP(BR)
      BBR=1.D0-DBR
      AR    =2.D0*R(I)*BBR*((DL2-1.D0)*BBR+BR*DJ2*DBR)
      AR    =AR   *F(I)**(-L1-L2)*BBR**(J1+J2-2)
      DR    =DL2*(1.D0-DL2)*BBR**2-2.D0*DJ2*(DL2-1.D0)*BR*DBR
     1 *BBR+DJ2*BR**2*DBR*(1.D0-DJ2*DBR)
      DR    =DR   *B(I)**(-L1-L2)*BBB**(J1+J2-2)
    1 CONTINUE
      IF(IJ.EQ.1) GO TO 5
      IF(II.EQ.1) GO TO 3
      F(I)=FQ(I)*(AR*DFP(I)+DR*FP(I))
      GO TO 10
    3 F(I)=FQ(I)*(AR*DGP(I)+DR*GP(I))
      GO TO 10
    5 IF(II.EQ.1) GO TO 7
      F(I)=GQ(I)*(AR*DFP(I)+DR*FP(I))
      GO TO 10
    7 F(I)=GQ(I)*(AR*DGP(I)+DR*GP(I))
   10 CONTINUE
      CALL DQB11(NM,DELR,F,Y)
      CEKIB=Y
      RETURN
    9 CEKIB=0.D0
      RETURN
      END
```

```
      FUNCTION CEXCH(II,P,L2,B2,J2,N,ZT,L,IJ,Q,L1,B1,J1,N,A,Z,LP,LQ)
C*****************************************************************************
C     COMPUTES RADIAL TWO-ELECTRON POTENTIAL (R<**L/R>**L+1)
C     CONTRIBUTION TO EXCHANGE FREE-FREE MATRIX ELEMENTS
C     THE FUNCTION ACTUALLY INVOLVES A DOUBLE INTEGRAL WHICH IS
C     EVALUATED NUMERICALLY FOR ALL COMBINATIONS OF II & IJ=0,1
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200),F(1200)
      COMMON/FFF/FP(1200),GP(1200),DFP(1200),DGP(1200),FQ(1200),GQ(1200)
      COMMON/BODE/DELR,R,NM
      COMMON/FIF/QF(1200),QG(1200)
      DO 2 I=1,NM
      QF(I)=FQ(I)
      QG(I)=GQ(I)
    2 CONTINUE
      DO 1 I=1,NM
      ZTR=-ZT*R(I)
      B2R=-B2*R(I)
      X=R(I)
      V=X**(N+2-L2)*DEXP(ZTR)*(X**(-L-1)*XIF(IJ,N+2+L-L1,J1,A,B1,I)-X**L
     1*XIF(IJ,N+1-L-L1,J1,A,B1,I))
      IF(J2.NE.0) V=V*(1.D0-DEXP(B2R))**J2
      IF(II.EQ.1) GO TO 3
      F(I)=V*FP(I)
      GO TO 1
    3 F(I)=GP(I)*V
    1 CONTINUE
      CALL DQB11(NM,DELR,F,Y)
      CEXCH=Y
    5 CEXCH=CEXCH+CTIB(II,N+2+L-L2,J2,ZT,B2,P,LP,FP,GP,Z)*
     * CTIB(IJ,N+1-L-L1,J1,A,B1,Q,LQ,FQ,GQ,Z)
      RETURN
      END
```

```
      FUNCTION CEXKE(II,ZT,L2,J2,B2,NZT,P,IJ,A,L1,J1,B1,NAT,Q,LA,LP,
     * E,Z)
C*************************************************************************
C     COMPUTES RADIAL SINGLE-PARTICLE-HAMILTONIAN CONTRIBUTION TO
C     EXCHANGE FREE-FREE MATRIX ELEMENTS
C     THE INTEGRAL IS EXPRESSED IN TERMS OF THE FUNCTION CTIB WHICH IS
C     EVALUATED NUMERICALLY FOR II(OR IJ)=1 AS THE INTEGRAND CONTAINS
C     THE IRREGULAR COULOMB FUNCTION
C*************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200)
      COMMON/BODE/DELR,R,NM
      COMMON/FFR/FP(1200),GP(1200),DFP(1200),DGP(1200),FQ(1200),GQ(1200)
      A1=-A**2
      A2=2.D0*(A*DFLOAT(NAT+1)-Z)
      A3=DFLOAT(LA*(LA+1)-NAT*(NAT+1))
      Z1=-(ZT**2+E)
      Z2=2.D0*(ZT*DFLOAT(NZT+1)-Z)
      Z3=DFLOAT(LP*(LP+1)-NZT*(NZT+1))
      F1=CTIB(IJ,NAT+2-L1,J1,A,B1,Q,LA,FQ,GQ,Z)
      F2=CTIB(II,NZT+2-L2,J2,ZT,B2,P,LP,FP,GP,Z)
      F3=CTIB(II,NZT-L2+1,J2,ZT,B2,P,LP,FP,GP,Z)
      F5=CTIB(IJ,NAT+1-L1,J1,A,B1,Q,LA,FQ,GQ,Z)
      CEXKE=(A1+Z1)*F1*F2+F1*Z2*F3+F2*A2*F5
      IF(NAT.EQ.LA.OR.NAT.EQ.(-LA-1)) GO TO 1
      CEXKE=CEXKE+F2*A3*CTIB(IJ,NAT-L1,J1,A,B1,Q,LA,FQ,GQ,Z)
    1 IF(NZT.EQ.LP.OR.NZT.EQ.(-LP-1)) RETURN
      CEXKE=CEXKE+F1*Z3*CTIB(II,NZT-L2,J2,ZT,B2,P,LP,FP,GP,Z)
      RETURN
      END
```

```
      SUBROUTINE CFFMX(FFD,FFX,SD,SX)
C*****************************************************************
C     COMPUTES DIRECT (FFD) AND EXCHANGE (FFX)  FREE FREE INTEGRALS :
C     MATRIX ELEMENTS OF (H-E) BETWEEN SLATER ORBITALS AND 2 REGULARIZED
C     FREE FUNCTIONS.H IS THE TOTAL HAMILTONIAN. E IS THE TOTAL ENERGY.
C     REQUIRES : CEXKE,CDIR,CEXCH,CEKID
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION FFD(2,2),FFX(2,2)
      DIMENSION SD(10,10),SX(10,10)
      DIMENSION  CEIG(5,10,10),NPWR(5,10),Z(5,10)
      DIMENSION ENRG(5,10),R(1200)
      COMMON/ABC/GAM,E,CEIG,Z,      P,Q,B,C,ENEG,L,LZ,LQ,LA,LP,NBSA,NBSZ
     1,NPWR,L2,L1,KB,JC,NA,NZ,NMAX,NZCH
      COMMON/RODE/DELR,R,NPTS
      COMMON/FFR/FP(1200),GP(1200),DFP(1200),DGP(1200),FQ(1200),GQ(1200)
      ZCH=DFLOAT(NZCH)
      JZ=LZ+1
      JA=LA+1
      DO 45 IIA=1,2
      II=IIA-1
      IF(II.EQ.0) J2=L2-1
      IF(II.EQ.1) J2=2*LP+L2
      DO 45 IJA=1,2
      IJ=IJA-1
      IF(IJ.EQ.0) J1=L1-1
      IF(IJ.EQ.1) J1=2*LQ+L1
      IF(IJA.EQ.1.AND.IIA.EQ.2.AND.JA.EQ.JZ.AND.NA.EQ.NZ.AND.L1.EQ.L2.
     1AND.LP.EQ.LQ) GO TO 30
      DO 15 I=1,NBSZ
      DCZ=DABS(CEIG(JZ,NZ,I))
      NZT=NPWR(JZ,I)
      TZ=Z(JZ,I)
      DO 15 J=1,NBSA
      DKX=0.0
      DPD=0.0
      DPX=0.0
      DCA=DABS(CEIG(JA,NA,J ))
      IF(DCZ.LT.1.0D-10)GO TO 14
      IF(DCA.LT.1.0D-10)GO TO 14
      NAT=NPWR(JA,J)
      TA=Z(JA,J)
      IF(LP.EQ.LZ.AND.LA.EQ.LQ) DKX=CEXKE(II,TZ,L2,J2,GAM,NZT,P,IJ,TA,L1,
     1J1,GAM,NAT,Q,LA,LP,E,ZCH)
      LLX=LA+LZ
      LLQ=LA+LQ
      LLP=LP+LZ
      LLY=LQ+LP
      LMX=MAXO(LLQ,LLX,LLY,LLP)+1
      DO 10 LL=1,LMX
      LM=LL-1
      QQ=ANGL(LM,L2,LQ,LA,LP,L)
      QN=DABS(QQ)
      IF(QN.LT.1.0D-08)GO TO 5
      DPD=DPD+QQ*CDIR(II,P,L2,GAM,J2,NZT,TZ,LM,IJ,Q,L1,GAM,J1,NAT,TA,
     1 LP,LQ,ZCH)
    5 QR=ANGL( LM,LQ,LZ,LA,LP,L)
      QX=DABS(QR)
      IF(QX.LT.1.0D-08)GO TO 10
      EXR=CEXCH(II,P,L2,GAM,J2,NZT,TZ,LM,IJ,Q,L1,GAM,J1,NAT,TA,ZCH,LP,LQ
```

```
     1)
      DPX=DPX+QR*SX(
   10 CONTINUE
   14 SD(I,J)=2.D0*DPD
   15 SX(I,J)=DKX+2.D0*DPX
      DS=0.0
      DX=0.0
      IF(LP.EQ.LQ.AND.LA.EQ.LZ.AND.NZ.EQ.NA) DS=CEKIB(IJ,II,J1,J2,L1,L2,L
     1P,GAM,Q,P)
      DO 21 NZ=1,NBSZ
      DCZ=DABS(CEIG(JZ,NZ,NZ))
      IF(DCZ.LT.1.0D-10)GO TO 21
      DO 20 NA=1,NBSA
      DCA=DABS(CEIG(JA,NA,NA))
      IF(DCA.LT.1.0D-10)GO TO 20
      DS=DS+CEIG(JZ,NZ,NZ)*SD(NZ,NA)*CEIG(JA,NA,NA)
      DX=DX+CEIG(JZ,NZ,NZ)*SX(NZ,NA)*CEIG(JA,NA,NA)
   20 CONTINUE
   21 CONTINUE
      FFD(IJA,IIA)=DS
      FFX(IJA,IIA)=DX
      GO TO 45
   30 FFX(IJA,IIA)=FFX(IIA,IJA)
      IF(LA.EQ.L2.AND.LP.EQ.LQ.AND.NZ.EQ.NA.AND.L1.EQ.1.AND.L2.EQ.1)GO
     1TO 35
      FFD(IJA,IIA)=FFD(IIA,IJA)
      GO TO 40
   35 FFD(IJA,IIA)=FFD(IIA,IJA)+P
   40 CONTINUE
   45 CONTINUE
      RETURN
      END
```

```
      FUNCTION CORINT(II,IJ,LP,LQ,P,Q,LM,Z,R)
C*****************************************************************
C     COMPUTES INTEGRALS OF THE TYPE : INT(R-INFINITY) OF
C     UASYMP(II,LP,EP,P*X) * UASYMP(IJ,LQ,EQ,Q*X) / X**(LM+1) ;LM=1,2,..
C     UASYMP IS A REGULAR(II,IJ=0) OR AN IRREGULAR(II,IJ=1) COULOMB FN.
C     EXPANDED IN THE ASYMPTOTIC REGION KEEPING POWERS OF X**(-3)
C     EP=-(Z-1)/P & EQ=-(Z-1)/Q , Z IS THE NUCLEAR CHARGE
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/CRH/PP,QQ,ZZ,RR,LLP,LLQ
      DIMENSION AP(5),BP(5),AQ(5),BQ(5)
      PP=P
      QQ=Q
      EP=-(Z-1.D0)/P
      EQ=EP*P/Q
      ZZ=Z
      RR=R
      LLP=LP
      LLQ=LQ
C
C     GENERATING THE EXPANSION COEFFICIENTS :
C
      DO 55 I=1,3
      K=I-1
      DK=K
      DKP=2.D0*(DK+1.D0)*P
      DKQ=2.D0*(DK+1.D0)*Q
      AP(I)=EP*(2.D0*DK+1.D0)/DKP
      BP(I)=(EP*EP+DFLOAT(LP*(LP+1)-K*(K+1)))/DKP
      AQ(I)=EQ*(2.D0*DK+1.D0)/DKQ
      BQ(I)=(EQ*EQ+DFLOAT(LQ*(LQ+1)-K*(K+1)))/DKQ
   55 CONTINUE
      A=AP(1)
      B=BP(1)
      C=AP(2)*A-B*BP(2)
      D=AP(2)*B+BP(2)*A
      E=AP(3)*C-BP(3)*D
      F=AP(3)*D+BP(3)*C
      AA=AQ(1)
      BB=BQ(1)
      CC=AQ(2)*AA-BQ(2)*BB
      DD=AQ(2)*BB+BQ(2)*AA
      EE=AQ(3)*CC-BQ(3)*DD
      FF=AQ(3)*DD+BQ(3)*CC
      A1=A+AA
      B1=BB
      C1=B
      A2=A*AA+C+CC
      B2=A*BB+DD
      C2=AA*B+D
      D2=B*BB
      A3=A*CC+C*AA+E+EE
      B3=A*DD+C*BB+FF
      C3=D*AA+B*CC+F
      D3=B*DD+D*BB
C
C     EVALUATING THE INTEGRALS FOR ALL COMBINATIONS OF II & IJ :
C
      IF(IJ.EQ.1)GO TO 2
      IF(II.EQ.1)GO TO 1
```

```
      CORINT=XCOR(0,0,LM)
      IF(DABS(CORINT).LE.1.D-08)RETURN
      FIRST=A1*XCOR(0,0,LM+1)+B1*XCOR(0,1,LM+1)+C1*XCOR(1,0,LM+1)
      CORINT=CORINT+FIRST
      IF(DABS(FIRST).LE.1.D-08)RETURN
      SECOND=A2*XCOR(0,0,LM+2)+B2*XCOR(0,1,LM+2)+C2*XCOR(1,0,LM+2)
     1       +D2*XCOR(1,1,LM+2)
      CORINT=CORINT+SECOND
      IF(DABS(SECOND).LE.1.D-08) RETURN
      THIRD=A3*XCOR(0,0,LM+3)+B3*XCOR(0,1,LM+3)+C3*XCOR(1,0,LM+3)
     1       +D3*XCOR(1,1,LM+3)
      CORINT=CORINT+THIRD
      RETURN
    1 CORINT=XCOR(1,0,LM)
      IF(DABS(CORINT).LE.1.D-08)RETURN
      FIRST=A1*XCOR(1,0,LM+1)+B1*XCOR(1,1,LM+1)-C1*XCOR(0,0,LM+1)
      CORINT=CORINT+FIRST
      IF(DABS(FIRST).LE.1.D-08)RETURN
      SECOND=A2*XCOR(1,0,LM+2)+B2*XCOR(1,1,LM+2)-C2*XCOR(0,0,LM+2)
     1       -D2*XCOR(0,1,LM+2)
      CORINT=CORINT+SECOND
      IF(DABS(SECOND).LE.1.D-08)RETURN
      THIRD=A3*XCOR(1,0,LM+3)+B3*XCOR(1,1,LM+3)-C3*XCOR(0,0,LM+3)
     1       -D3*XCOR(0,1,LM+3)
      CORINT=CORINT+THIRD
      RETURN
    2 IF(II.EQ.1)GO TO 3
      CORINT=XCOR(0,1,LM)
      IF(DABS(CORINT).LE.1.D-08)RETURN
      FIRST=A1*XCOR(0,1,LM+1)-B1*XCOR(0,0,LM+1)+C1*XCOR(1,1,LM+1)
      CORINT=CORINT+FIRST
      IF(DABS(FIRST).LE.1.D-08)RETURN
      SECOND=A2*XCOR(0,1,LM+2)-B2*XCOR(0,0,LM+2)+C2*XCOR(1,1,LM+2)
     1       -D2*XCOR(1,0,LM+2)
      CORINT=CORINT+SECOND
      IF(DABS(SECOND).LE.1.D-08)RETURN
      THIRD=A3*XCOR(0,1,LM+3)-B3*XCOR(0,0,LM+3)+C3*XCOR(1,1,LM+3)
     1         -D3*XCOR(1,0,LM+3)
      CORINT=CORINT+THIRD
      RETURN
    3 CORINT=XCOR(1,1,LM)
      IF(DABS(CORINT).LE.1.D-08)RETURN
      FIRST=A1*XCOR(1,1,LM+1)-B1*XCOR(1,0,LM+1)-C1*XCOR(0,1,LM+1)
      CORINT=CORINT+FIRST
      IF(DABS(FIRST).LE.1.D-08)RETURN
      SECOND=A2*XCOR(1,1,LM+2)-B2*XCOR(1,0,LM+2)-C2*XCOR(0,1,LM+2)
     1       +D2*XCOR(0,0,LM+2)
      CORINT=CORINT+SECOND
      IF(DABS(SECOND).LE.1.D-08)RETURN
      THIRD=A3*XCOR(1,1,LM+3)-B3*XCOR(1,0,LM+3)-C3*XCOR(0,1,LM+3)
     1    +D3*XCOR(0,0,LM+3)
      CORINT=CORINT+THIRD
      RETURN
      END
```

```
      SUBROUTINE CSEX2(R,Q,N,INVR,NMAX,R,XXS,YYS,CCQ,DDQ)
C*****************************************************************
C     WRITTEN BY DR J. CALLAWAY .REVISED FEB. 1976
C     COMPUTES CROSS SECTIONS FROM THE REACTANCE (R) MATRIX
C      RETURNS REAL (XXS) AND IMAGINARY (YYS) PARTS OF THE TRANSITION
C      AMPLITUDE MATRIX TO THE CALLING PROGRAM
C     REQUIRES SUBROUTINE GMIC2
C     N IS THE NUMBER OF CHANNELS
C     INVR=0,1 FOR SINGLET AND TRIPLET ELEMENTS RESPECTIVELY
C     NMAX IS THE MAXIMUM DIMENSION OF THE R-MATRIX
C     REMARK : FUNCTIONS DIMAG & DAIMAG ARE EQUIVALENT (THEY BOTH
C              FIND THE IMAGINARY PART OF A COMPLEX NUMBER).
C*****************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION R(NMAX,NMAX),Q(NMAX,NMAX),XXS(NMAX,NMAX),YYS(NMAX,NMAX)
      COMPLEX*16 B(NMAX,NMAX),Z,ZA,CCQ(NMAX,NMAX),DDQ(NMAX)
      IF(INVR.GE.1)GO TO 4
      DO 1 I=1,N
      DO 1 J=1,N
      X=0.0
      IF(I.EQ.J)X=1.0
      Y=-R(I,J)
    1 B(I,J)=DCMPLX(X,Y)
      CALL GMIC2(N,B,NMAX,CCQ,DDQ)
      DO 3 I=1,N
      DO 3 J=1,N
      Z=0.0
      DO 2 K=1,N
      ZA=R(I,K)
    2 Z=Z+ZA*B(K,J)
      X=DREAL(Z)
      Y=DAIMAG(Z)
      XXS(I,J)=X
      YYS(I,J)=Y
    3 Q(I,J)=X*X+Y*Y
      RETURN
    4 DO 5 I=1,N
      DO 5 J=1,N
      Y=0.0
      IF(I.EQ.J)Y=-1.0
      X=R(I,J)
    5 B(I,J)=DCMPLX(X,Y)
      CALL GMIC2(N,B,NMAX,CCQ,DDQ)
      DO 6 I=1,N
      DO 6 J=1,N
      Z=B(I,J)
      X=DREAL(Z)
      Y=DAIMAG(Z)
      XXS(I,J)=X
      YYS(I,J)=Y
    6 Q(I,J)=X*X+Y*Y
      RETURN
      END
```

```
      FUNCTION CTIB(II,LP,J,X,B,P,L,F,G,Z)
C*****************************************************************************
C     EVALUATES INTEGRALS OF THE TYPE : INT(0-INFINITY) OF
C        (R**LP)*EXP(-X*R)*((1-EXP(-B*R))**J)*U(L,P*R)
C     U IS EITHER THE REGULAR(F) OR IRREGULAR(G) COULOMB FUNCTION
C     Z IS THE NUCLEAR CHARGE & AX=-(Z-1)/P IS THE COULOMB PARAMETER
C     THE INTEGRAL IS EVALUATED NUMERICALLY FOR II=1 (U=G)
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200),F(1200),G(1200),H(1200)
      COMMON/BODE/DR,R,NM
      COMMON/ANL/TK,AX
      TK=P
      AX=-(Z-1.D0)/P
      IF(II.EQ.0.AND.LP.LT.(-L-1))GO TO 6
      IF(II.EQ.1 )GO TO 6
      IF(J.GT.0)GO TO 1
      CTIB=XLJ(L,LP,X)
      RETURN
    1 J1=J+1
      CTIB=0.D0
      DPJ=DFACTR(J)
      DO 2 N=1,J1
      M=N-1
    2 CTIB=CTIB+(-1.D0)**M*XLJ(L,LP,X+B*DFLOAT(M))/(DFACTR(M)*
     1           DFACTR(J-M))
      CTIB=CTIB*DPJ
      RETURN
    6 DO 7 I=1,NM
      V=R(I)**LP*DEXP(-X*R(I))
      IF(J.NE.0)V=V*(1.D0-DEXP(-B*R(I)))**J
      IF(II.EQ.0)H(I)=V*F(I)
      IF(II.EQ.1)H(I)=V*G(I)
    7 CONTINUE
      CALL DQB11(NM,DR,H,YY)
      CTIB=YY
      RETURN
      END
```

```
      FUNCTION DFACTR(N)
C*****************************************************************************
C     GENERATES N!  WITH AN ASYMPTOTIC FORMULA FOR N GE 41
C     NOTE : FUNCTION FACTR(N) IS ANOTHER DOUBLE PRECISION VERSION
C            THAT HAS BEEN WRITTEN BY DR J. CALLAWAY
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION FCT(40)
      IF(N.LT.0) RETURN
      IF(N.EQ.0)  GO TO 30
      FCT(1)=1.D0
      IF (N.EQ.1) GO TO 30
      IF(N.GE.41)  GO TO 20
      DO 10 IN=2,N
      DN=DFLOAT(IN)
   10 FCT(IN)=FCT(IN-1)*DN
      DFACTR=FCT(N)
      GO TO 40
   20 XN=DFLOAT(N)
      PI=3.1415926535897930D00
      E=2.7182818284590450D00
      PIN=2.D0*XN*PI
      XN1=12.D0*XN
      XN2=288.D0*(XN**2)
      DFT=DSQRT(PIN)*((XN/E)**N)*(1.D0+(1.D0/XN1)+(1.D0/XN2))
      DFACTR=DFT
      GO TO 40
   30 DFACTR=1.D0
   40 RETURN
      END
```

```
      SUBROUTINE DQD11(N,H,F,FNS)
C*****************************************************************************
C     COMPUTES INTEGRALS USING THE 11PT. NEWTON-COTE CLOSED TYPE
C     FORMULA WITH FIXED MESH SIZE
C     N IS THE NUMBER OF MESHES (N=10*M+1,WHERE M=1,2,3,....)
C     H IS THE MESH SIZE
C     F IS THE INPUT VECTOR FUNCTION
C     FNS IS THE ESTIMATED INTEGRAL WITH AN ERROR OF THE ORDER OF H**13
C     REMARK: THE MESH SIZE DOES NOT HAVE TO BE VERY SMALL
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION W(6),F(1200)
      W(1)=16067.D0
      W(2)=106300.D0
      W(3)=-48525.D0
      W(4)=272400.D0
      W(5)=-260550.D0
      W(6)=427363.D0
      V=5.D0*H/299376.D0
      SUM1=0.D0
      SUM2=0.D0
      SUM3=0.D0
      M=(N-1)/10
      M1=M-1
      DO 1 I=1,M1
    1 SUM1=SUM1+2.D0*F(1+10*I)
      DO 4 I=2,6
      SUM4=0.D0
      DO 3 K=1,M
    3 SUM4=SUM4+F(  I+10*(K-1))
      SUM2=SUM2+W(I)*SUM4
    4 CONTINUE
      DO 5 I=2,5
      SUM5=0.D0
      DO 2 K=1,M
    2 SUM5=SUM5+F(2+10*K-I)
    5 SUM3=SUM3+W(I)*SUM5
      FNS=W(1)*     (F(1)+F(N)+SUM1)+SUM2+SUM3
      FNS=FNS*V
      RETURN
      END
```

```
      DOUBLE PRECISION FUNCTION F6J(JD1,JD2,JD3,LD1,LD2,LD3)
C*****************************************************************************
C     WRITTEN BY DR. J. CALLAWAY
C     F6J FUNCTION CALLS S6J (VERSION II FORTRAN IV)
C     ANGULAR MOMENTUM COUPLING TESTS FOR 6J COEFFICIENT
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION MED(12)
      J1=JD1
      J2=JD2
      J3=JD3
      L1=LD1
      L2=LD2
      L3=LD3
      I=-J1+J2+J3
      I1=I/2
      IF (I-2*I1) 1000,1010,1000
 1000 F6J=0.0
      GO TO 100
 1010 MED(1)=I1
      I=+J1-J2+J3
      I1=I/2
      IF (I-2*I1) 1000,1020,1000
 1020 MED(2)=I1
      I=+J1+J2-J3
      I1=I/2
      IF (I-2*I1) 1000,1030,1000
 1030 MED(3)=I1
      I=-J1+L2+L3
      I1=I/2
      IF (I-2*I1) 1000,1040,1000
 1040 MED(4)=I1
      I=+J1-L2+L3
      I1=I/2
      IF (I-2*I1) 1000,1050,1000
 1050 MED(5)=I1
      I=+J1+L2-L3
      I1=I/2
      IF (I-2*I1) 1000,1060,1000
 1060 MED(6)=I1
      I=-L1+J2+L3
      I1=I/2
      IF (I-2*I1) 1000,1070,1000
 1070 MED(7)=I1
      I=+L1-J2+L3
      I1=I/2
      IF (I-2*I1) 1000,1080,1000
 1080 MED(8)=I1
      I=+L1+J2-L3
      I1=I/2
      IF (I-2*I1) 1000,1090,1000
 1090 MED(9)=I1
      I=-L1+L2+J3
      I1=I/2
      IF (I-2*I1) 1000,1100,1000
 1100 MED(10)=I1
      I=+L1-L2+J3
      I1=I/2
      IF (I-2*I1) 1000,1110,1000
 1110 MED(11)=I1
```

```
      I=+L1+L2-J3
      I1=I/2
      IF (I-2*I1) 1000,1120,1000
 1120 MED(12)=I1
      DO 10 N=1,12
      IF (MED(N)) 1000,10,10
   10 CONTINUE
      P6J=S6J(J1,J2,J3,L1,L2,L3)
  100 RETURN
      END
```

```
      FUNCTION GK(L,R,P,Q)
C*****************************************************************
C     COMPUTES INTEGRALS OF THE TYPE : INT(R-INFINITY) OF
C              EXP(I*Q*X) / X**(L+1+I*P)
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      COMPLEX*16 U,GK,PQR,QRL,SUM,PROD,SUMM,RQ,QR
      IF(DABS(P).LE.1.D-06.AND.DABS(Q).LE.1.D-06.AND.L.GE.1) GO TO 10
      U=DCMPLX(0.D0,1.D0)
      PQR=DCMPLX(0.D0,Q*R-P*DLOG(R))
      QRL=DCMPLX(Q*R**(L+1),0.D0)
      GK=U*CDEXP(PQR)/QRL
      IF(CDABS(GK).LE.1.D-08) RETURN
      NT=30
      QR=DCMPLX(0.D0,Q*R)
      SUMM=DCMPLX(1.D0,0.D0)
      DO 2 N=1,NT
      PROD=DCMPLX(1.D0,0.D0)
      DO 1 J=1,N
      PROD=PROD*DCMPLX(DFLOAT(L+J),P)
    1 CONTINUE
      SUM=PROD/(QR**N)
      IF(CDABS(SUM).LE.1.D-08) GO TO 3
    2 SUMM=SUMM+SUM
      GO TO 4
    3 SUMM=SUMM+SUM
    4 GK=GK*SUMM
      RETURN
   10 GK=DCMPLX(1.D0/(DFLOAT(L)*(R**L)),0.D0)
      RETURN
      END
```

```
      SUBROUTINE GMIC2(L,B,LMAX,C,D)
C*****************************************************************************
C     WRITTEN BY DR J. CALLAWAY. REVISED FEB. 1976
C     L = DIMENSION OF ACTUAL MATRIX TO BE INVERTED
C      B = MATRIX TO BE INVERTED.  B IS REPLACED BY ITS INVERSE.
C     LMAX IS THE MAXIMUM DIMENSION OF THE ARRAYS B,C,&D
C     THE ENTRIES OF B MAY BE COMPLEX
C*****************************************************************************
      COMPLEX*16 B(LMAX,LMAX),C(LMAX,LMAX),D(LMAX),Q
      DO 1 N=1,L
      DO 1 M=1,L
    1 C(N,M)=0.0
      DO 5 N=1,L
      DO 5 M=1,L
      Q=B(N,M)
      DO 2 J=1,L
    2 Q=Q-C(N,J)*C(J,M)
      IF(N-M)4,3,3
    3 C(N,M)=Q
      GO TO 5
    4 C(N,M)=Q/C(M,M)
    5 CONTINUE
      DO 6 N=1,L
      DO 6 M=1,L
    6 B(N,M)=0.0
      DO 11 N=1,L
      DO 7 M=1,L
    7 D(M)=0.0
      D(N)=1.
      DO 9 M=1,L
      Q=D(M)
      DO 8 J=1,L
      IF(J-M)8,9,9
    8 Q=Q-C(M,J)*D(J)
    9 D(M)=Q/C(M,M)
      DO 11 MM=1,L
      M=L+1-MM
      Q=D(M)
      DO 10 JJ=1,L
      J=L+1-JJ
   10 Q=Q-C(M,J)*B(J,N)
   11 B(M,N)=Q
      RETURN
      END
```

```
      SUBROUTINE GMIS(L,B,C,D,DET,LMAX)
C*****************************************************************************
C     WRITTEN BY DR J. CALLAWAY
C     L IS ACTUAL DIMENSION OF MATRIX,  LMAX IS MAXIMUM DIMENSION
C      INVERTS  AN ORDINARY MATRIX B.  DET IS THE DETERMINANT
C     B IS REPLACED BY ITS INVERSE
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION B(LMAX,LMAX),C(LMAX,LMAX),D(LMAX)
      DO 1 N=1,L
      DO 1 M=1,L
    1 C(N,M)=0.0
      DO 5 N=1,L
      DO 5 M=1,L
      Q=B(N,M)
      DO 2 J=1,L
    2 Q=Q-C(N,J)*C(J,M)
      IF(N-M)4,3,3
    3 C(N,M)=Q
      GO TO 5
    4 C(N,M)=Q/C(M,M)
    5 CONTINUE
      DET=1.0
      DO 51 M=1,L
   51 DET=DET*C(M,M)
      DO 6 N=1,L
      DO 6 M=1,L
    6 B(N,M)=0.0
      DO 11 M=1,L
      DO 7 N=1,L
    7 D(N)=0.0
      D(M)=1.0
      DO 9 N=1,L
      Q=D(N)
      DO 8 J=1,L
      IF(J-N)8,9,9
    8 Q=Q-C(N,J)*D(J)
    9 D(N)=Q/C(N,M)
      DO 11 NN=1,L
      N=L+1-NN
      Q=D(N)
      DO 10 JJ=1,L
      J=L+1-JJ
   10 Q=Q-C(N,J)*B(J,M)
      B(N,M)=Q
   11 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE KRO2(BBQ,CCQ,DDQ,ISKP,
     1                TKS,FFAS,ALPO,BETO,RM,RIM,QCR,QCI,RJM,C,D,XXS,
     2YYS,XXT,YYT,RKK,RIR,LAT,NCHMX,KMX,KMMAX,IWRT,NE,IEIPH,NPST,KPUN)
C*********************************************************************
C     WRITTEN BY DR J. CALLAWAY. REVISED FEB. 1981
C     COMPUTES REACTANCE (OR K-) MATRIX ELEMENTS ON THE BASIS OF THE
C     'ALGEBRAIC VARIATIONAL METHOD' USING THE KOHN & INVERSE-KOHN
C     FORMULAS.
C*********************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION TKS(NCHMX),LAT(NCHMX)
      DIMENSION FFAS(KMX,2,KMX,2)
      DIMENSION ALPO(KMX,KMX),BETO(KMX,KMX),RM(KMX,KMX),RIM(KMX,KMX),QCR
     1(KMX,KMX),QCI(KMX,KMX),RJM(KMX,KMX),C(KMX,KMX),D(KMX),XXS(KMX,KMX)
     2,XXT(KMX,KMX),YYS(KMX,KMX),YYT(KMX,KMX)
      DIMENSION RKK(KMMAX),RIR(KMMAX)
      COMPLEX*16 BBQ(KMX,KMX),CCQ(KMX,KMX),DDQ(KMX)
      PI=3.141592653589790
C
C.....................CONTROL VARIABLES.............................
C     IF IWRT.EQ.1 TKS AND LAT ARE PRINTED
C     TKS & LAT ARE THE CHANNEL ENERGIES AND TARGET ANGULAR MOMENTA.
C     IF IWRT.GE.2     K MATRICES  AND CROSS SECTIONS ARE PRINTED
C     IF IEIPH EQ 0, EIGENPHASES ARE NOT CALCULATED
C     IF KPUN GE. 10 KOHN & IN.-KOHN K-MATRIX ELEMENTS ARE STORED ON
C     UNITS KPUN & KPUN+1 RESPECTIVELY.
C     IF KPUN=7 BOTH TYPES OF ELEMENTS ARE PUNCHED ON CARDS.
C     IF ISKP GT 0 K-MATRICES ARE NEITHER  STORED NOR PUNCHED
C     NE IS THE NUMBER OF ENERGIES (USUALLY NE=1)
C     NPST=NUMBER OF PSEUDOSTATES IN SET: 3 FOR 3S-3P,8 FOR 6S-5P-2D-1F
C     KMX MUST AGREE WITH  DIMENSIONS OF ALPO ETC
C
      K2=KMX*KMX
  100 FORMAT(I5)
      DO 91 IE=1,NE
C
C     READS IN CHANNEL PARAMETERS :
C
      READ(8)IA,IB,IC,NCH,KCHT,LMX,L,NDIM
      READ(8)(TKS(I),I=1,KCHT)
      READ(8)(LAT(I),I=1,KCHT)
      E=TKS(1)*TKS(1)
  101 FORMAT(15X,2I5,5X,I5)
      WRITE(6,222)
  222 FORMAT(1X,'TOTAL ANGULAR MOMENTUM',2X,'INCIDENT ENERGY',2X,'# OF
     1OPEN CHANNELS',2X,'TOTAL # OF CHANNELS',1X/)
      WRITE(6,105)
      WRITE(6,104) L,E,NCH,KCHT
  104 FORMAT(7X,I5,11X,F15.7,9X,I5,16X,I5)
      WRITE(6,105)
      WRITE(6,233)
  233 FORMAT(1X'ANGULAR MOMENTA OF PSEUDOSTATES : ',1X/)
      IF(IWRT.GE.1)WRITE(6,102)(LAT(I) ,I=1,KCHT)
  102 FORMAT(19I4)
      WRITE(6,105)
      WRITE(6,333)
  333 FORMAT(1X,'CHANNEL ENERGIES : ',1X/)
      IF(IWRT.GE.1)WRITE(6,202)(I,TKS(I),I=1,KCHT)
  202 FORMAT(I5,F19.14)
      DO 90 IAS=1,2
```

```
      WRITE(6,105)
      IF(IAS.EQ.1) WRITE(6,444)
      IF(IAS.EQ.2) WRITE(6,555)
  444 FORMAT('  SINGLET',1X)
  555 FORMAT('  TRIPLET',1X)
      WRITE(6,105)
  105 FORMAT(1H )
C
C     READS IN M-MATRIX ELEMENTS :
C
      DO 1 ICH=1,NCH
      DO 1 IIA=1,2
      DO 1 JCH=1,NCH
      DO 1 JJA=1,2
    1 READ(4) IA,IB,IC,ID,FFAS(IA,IB,IC,ID)
      IF(NCH.EQ.1) GO TO 62
      DO 61 I=1,NCH
      DO 61 J=1,NCH
      RM (I,J)=FFAS(I,2,J,2)
   61 RIM(I,J)=FFAS(I,1,J,1)
C
C     STARTS EVALUATING REACTANCE MATRICES :
C
      CALL GMIS(NCH,RM ,C,D,DDDB,KMX)
      CALL GMIS(NCH,RIM,C,D,DDDA,KMX)
      WRITE(6,666)
  666 FORMAT(1X,'DETM :',9X,'KOHN',12X,'INVERSE KOHN',1X/)
      WRITE(6,210) DDDA,DDDB
  210 FORMAT(5X,2D21.9)
      GO TO 63
   62 RM (1,1)=1.D0/FFAS(1,2,1,2)
      RIM(1,1)=1.D0/FFAS(1,1,1,1)
   63 DO 65 I=1,NCH
      DO 65 J=1,NCH
      ALFO(I,J)=0.0
      BETO(I,J)=0.0
      DO 64 K=1,NCH
      ALFO(I,J)=ALFO(I,J)-RM (J,K)   *FFAS(K,2,I,1)
   64 BETO(I,J)=BETO(I,J)-RIM (J,K)*FFAS(K,1,I,2)
   65 CONTINUE
      DO 69 I=1,NCH
      DO 67 J=1,NCH
      RM  (I,J)=FFAS(J,1,I,1)
      RIM (I,J)=FFAS(J,2,I,2)
      DO 66 K=1,NCH
      RM  (I,J)=RM  (I,J)+FFAS(K,2,J,1)*ALFO(I,K)
   66 RIM (I,J)=RIM (I,J)+FFAS(K,1,J,2)*BETO(I,K)
   67 CONTINUE
      K=0
      DO 68 J=1,NCHT
      IF(TKS(J).LT.0.0) GO TO 681
      K=K+1
      RM (I,K)=-RM(I,K)/TKS(J)
      RIM(I,K)=RIM(I,K)/TKS(J)
  681 CONTINUE
   68 CONTINUE
   69 CONTINUE
      WRITE(6,105)
      K=0
      IF(NCH.GT.1) GO TO 70
```

```
      DKN2=DATAN(RM(1,1))
      TRB2=1.D0/RIM(1,1)
      DRB2=DATAN(TRB2)
      IF(L.EQ.0.AND.DKN2.LE.0.0) DKN2=DKN2+PI
      IF(L.EQ.0.AND.DRB2.LE.0.0) DRB2=DRB2+PI
      WRITE(6,777)
  777 FORMAT(1X,'SINGLE CHANNEL SCATTERING PHASE SHIFTS(RADS.),KOHN,INVE
     1RSE KOHN',1X//)
      WRITE(6,210) DKN2,DRB2
      GO TO 90
   70 DO 72 I=1,KCHT
      IF(TKS(I).LT.0.0) GO TO 72
      K=K+1
      M=0
      DO 71 J=1,KCHT
      IF(TKS(J).LT.0.0) GO TO 71
      M=M+1
      QQ=TKS(J)/TKS(I)
      QQ=DSQRT(QQ)
      RM (K,M)=QQ*RM (K,M)
      RIM(K,M)=QQ*RIM(K,M)
      RJM(K,M)=RIM(K,M)
   71 CONTINUE
   72 CONTINUE
      CALL GMIS(NCH,RJM,C,D,DDQ,KNX)
      WRITE(6,888)
  888 FORMAT(1X,'K MATRIX',12X,'KOHN',13X,'INVERSE KOHN',1X/)
      DO 721 I=1,NCH
      IF(IWRT.LE.1.AND.I.NE.1) GO TO 721
      DO 721 J=1,NCH
      WRITE(6,107) I,J,RM(I,J),RJM(I,J)
  721 CONTINUE
  107 FORMAT(2I5,2F21.9)
C
C     STORES (OR PUNCHES) REACTANCE MATRICES :
C
      IF(KPUN.LE.0) GO TO 750
      IF(ISKP.EQ.1.AND.IAS.EQ.2)GO TO 750
      IF(ISKP.EQ.2.AND.IAS.EQ.1)GO TO 750
      KPUN1=KPUN+1
      IF(KPUN.EQ.7) KPUN1=KPUN
      WRITE(KPUN,111) E
      DO 748 I=1,NCH
      DO 748 J=I,NCH
  748 WRITE(KPUN,110) I,J,RM(I,J)
      WRITE(KPUN1,111) E
  111 FORMAT(F15.10)
      DO 749 I=1,NCH
      DO 749 J=I,NCH
  749 WRITE(KPUN1,110) I,J,RJM(I,J)
  750 CONTINUE
  110 FORMAT(2I5,F17.10)
      WRITE(6,105)
C
C     CALCULATES EIGENPHASES AND SPIN WEIGHTED PARTIAL SCATTERING
C     CROSS-SECTIONS :
C
  722 CALL CSEK2(RM,QCR,NCH,0,KNX,BBQ,XXS,YYS,CCQ,DDQ)
      CALL CSEK2(RIM,QCI,NCH,1,KNX,BBQ,XXT,YYT,CCQ,DDQ)
      I=1
```

```
      WRITE(6,999)
  999 FORMAT(1X,'T MATRIX ELEMENTS',12X,'KOHN',40X,'INVERSE KOHN',1X/
     119X,'REAL PART',9X,'IMAGINARY PART',18X,'REAL PART',10X,'IMAGINARY
     2 PART',1X//)
      DO 723 J=1,NCH
  723 WRITE(6,724)I,J,XXS(I,J),YYS(I,J),XXT(I,J),YYT(I,J)
  724 FORMAT(2I5,2D21.9,10X,2D21.9)
      WRITE(6,105)
      IF(IEIPH.EQ.0)GO TO 727
      DO 725 I=1,NCH
      DO 725 J=I,NCH
      KIJ=I+(J*(J-1))/2
      RKK(KIJ)=(R_M(I,J)+R_M(J,I))/2.DO
  725 RIR(KIJ)=(RJM(I,J)+RJM(J,I))/2.DO
      CALL SIGEN(RKK,XXT,NCH,0,K2,KMMAX)
      CALL SIGEN(RIR,YYT,NCH,0,K2,KMMAX)
      SUMK=0.0DO
      SUMR=0.0DO
      WRITE(6,2222)
 2222 FORMAT(1X,'IGENPHASES :',5X,'KOHN',10X,'INVERSE KOHN',1X//)
      DO 726 I=1,NCH
      KII=I+(I*(I-1))/2
      STK=DATAN(RKK(KII))
      STR=DATAN(RIR(KII))
      SUMR=SUMR+STR
      SUMK=SUMK+STK
  726 WRITE(6,106)I,STK,STR
      WRITE(6,105)
      WRITE(6,3333)
 3333 FORMAT(5X,'IGENPHASE SUMS',1X//)
      WRITE(6,109)SUMK,SUMR
  106 FORMAT(I5,2D21.9)
  109 FORMAT(5X,2D21.9)
      WRITE(6,105)
  727 CONTINUE
      ALQA=2.0*FLOAT(L)+1.0
      ALQC=1.0
      IF(IAS.EQ.2)ALQC=3.0
      I=0
      WRITE(6,4444)
 4444 FORMAT(1X,'CROSS SECTIONS',6X,'KOHN',13X,'INVERSE KOHN',1X//)
      DO 74 K=1,KCHT
      IF(TKS(K).LT.0.0)GO TO 74
      ALQB=2.0*FLOAT(LAT(K))+1.0
      PPQ=ALQA*ALQC/(ALQB*TKS(K)*TKS(K))
      I=I+1
      DO 73 J=1,NCH
      QCR(I,J)=QCR(I,J)*PPQ
      QCI(I,J)=QCI(I,J)*PPQ
      IF(IWRT.LE.1.AND.I.NE.1)GO TO 731
      WRITE(6,108)I,J,QCR(I,J),QCI(I,J)
  108 FORMAT(2I5,2D21.9)
      GO TO 73
  731 CONTINUE
   73 CONTINUE
      IF(I.EQ.1)WRITE(6,105)
   74 CONTINUE
   90 CONTINUE
   91 CONTINUE
      REWIND 8
```

```
REWIND 4
RETURN
END
```

```
C     DRIVING PROGRAM 1. GENERATES VARIATIONAL MATRIX ELEMENTS
C     FOR ELECTRON SCATTERING BY HYDROGENLIKE IONS
C
C*****************************************************************
C     CALLS SUBROUTINE MPT1K WHICH EVALUATES THE BOUND-BOUND,
C     BOUND-FREE,AND FREE-FREE MATRIX ELEMENTS
C     MCHMX IS THE MAXIMUM NUMBER OF CHANNELS
C     MCAT IS THE MAXIMUM NUMBER OF OPEN CHANNELS
C     MDMX IS THE MAXIMUM NUMBER OF ELEMENTS IN THE PSEUDOBASIS
C     IF MDMX NE 10, DIMENSIONS OF SD AND SX, ETC IN SUBROUTINE MPT1K
C     MUST BE CHANGED
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION LCH(40),TKS(40),LAT(40),KAT(40)
      DIMENSION BFAS(466,40,2),BFAT(466,40,2)
      DIMENSION FFAS(40,2,40,2),FFAT(40,2,40,2)
      MBIG=466
      MDMX=10
      READ(5,100)MCHMX,MCAT
  100 FORMAT(2I5)
      WRITE(6,100)MCHMX,MCAT
      CALL MPT1K(BFAS,BFAT,FFAS,FFAT,TKS,LCH,LAT,KAT,MCHMX,
     1MCAT,MBIG,MDMX)
      STOP
      END
```

```
C     DRIVING PROGRAM 2. GENERATES M-MATRIX ELEMENTS
C
C*****************************************************************
C     CALLS SUBROUTINE MPT2C WHICH INVERTS THE BOUND-BOUND MATRIX
C     AND GENERATES THE M-MATRIX ELEMENTS GIVEN BY:
C       M=FF - BF * (1/BB) * DF
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION TKS(40)
      DIMENSION BFAS(466,40,2),BFAT(466,40,2)
      DIMENSION B(108811),D(466)
      DIMENSION FFAS(40,2,40,2),FFAT(40,2,40,2)
      NCAT=40
      NCHMI=40
      NBIG=466
      NGND=466
      NGMM=(NGND*(NGND+1))/2
  100 FORMAT(5L5)
      CALL       MPT2C(BFAS,BFAT,FFAS,FFAT,B,D,TKS,NGMM,NGND,NBIG,NCAT,
     1NCHMI)
      STOP
      END
```

```
C     DRIVING PROGRAM 3. GENERATES KOHN & INVERSE-KOHN  K-MATRICES
C
C*********************************************************************
C      CALLS KRO2 WHICH EVALUATES K-(OR R-) MATRIX ELEMENTS USING
C      THE KOHN AND INVERSE KOHN  FORMULAS.IT ALSO EVALUATES
C      EIGENPHASES,T-MATRIX ELEMENTS AND SCATTERING CROSS-SECTIONS
C*********************************************************************
       IMPLICIT REAL*8(A-H,O-Z)
       DIMENSION TKS(40),LAT(40)
       DIMENSION FFAS(40,2,40,2)
       COMMON/WDR/
      1          ALFO(40,40),BETO(40,40),RM(40,40),RIM(40,40),QCR(40,40),
      2QCI(40,40),RJM(40,40),C(40,40),D(40)
      3,         XXS(40,40),YYS(40,40),XXT(40,40),YYT(40,40)
       DIMENSION RKR(820),RIR(820)
       COMPLEX*16 BBQ(40,40),CCQ(40,40),DDQ(40)
       EQUIVALENCE(RKR(1),XXS(1,1))
       EQUIVALENCE(RIR(1),YYS(1,1))
       READ(5,101)IWRT,NE,IEIPH
       READ(5,101)NPST,KPUN,ISKP
C
C      THE CONTROL PARAMETERS IWRT,IEIPH,ISKP,AND KPUN ARE DEFINED
C      IN SUBROUTINE KRO2
C      NE IS THE NUMBER OF TOTAL ENERGIES AT WHICH THE PROGRAM IS RUN
C      NPST IS THE NUMBER OF PSEUDOSTATES
C
       NCHMX=40
       KMX=40
       KMMAX=(KMX*(KMX+1))/2
       CALL KRO2(BBQ,CCQ,DDQ,ISKP,
      1              TKS,FFAS,ALFO,BETO,RM,RIM,QCR,QCI,RJM,C,D,XXS,YYS,XXT
      2,YYT,RKR,RIR,LAT,NCHMX,KMX,KMMAX,IWRT,NE,IEIPH,NPST,KPUN)
  101 FORMAT(3I5)
       STOP
       END
```

```
C     DRIVING PROGRAM 4. GENERATES OMN & IOMN K-MATRICES
C
C*****************************************************************************
C     CALLS OMN2 WHICH EVALUATES K-MATRIX ELEMENTS USING THE OMN & IOMN
C     FORMULAS. IT ALSO CALCULATES EIGENPHASES,T-MATRIX ELEMENTS AND
C     SCATTERING CROSS-SECTIONS
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION TKS(40),LAT(40),TKN(40),TNN(40),LNN(40)
      DIMENSION PPAS(40,2,40,2),BO(40,40),B1(40,40),XXS(40,40),YYS(40,40
     1),A(80,80),U(80,80),TM(80,80),AX(6400),AO(40,40),A1(40,
     240),RO(40,40),ROS(820)   ,CD(40),SD(40),SMD(40,40),CMD(40,40),PMOO
     3(40,40),PM11(40,40),PM10(40,40),PR(40,40),SCR(40,40),FR(
     440,40),CSX(40,40),CSR(1600),EMTM(3240),LXN(40),TXN(40)
      COMPLEX*16 BBQ(40,40),CCQ(40,40),DDQ(40,40)
      EQUIVALENCE(PM10(1,1),PR(1,1))
      EQUIVALENCE(ROS(1),PM11(1,1))
      EQUIVALENCE(RO(1,1),PMOO(1,1))
      EQUIVALENCE(AO(1,1),PR(1,1))
      EQUIVALENCE(CSX(1,1),CSR(1))
      EQUIVALENCE(U(1,1),AX(1))
      EQUIVALENCE(TKN(1),TNN(1))
      EQUIVALENCE(EMTM(1),TM(1,1))
      KNX=40
      K2=KNX*KNX
      KNLM=2*KNX
      NMAX=(KNLM*(KNLM+1))/2
      N2=4*K2
      KNMAX=(KNX*(KNX+1))/2
      NCHMX=40
      READ(5,100)NWRT,NPUN,NE,ICSWT,IOMN
      READ(5,100)NPST,KPUN,ISKP
C
C     THE CONTROL PARAMETERS NWRT,NPUN,ICWST,IOMN,KPUN,& ISKP ARE
C     DEFINED IN SUBROUTINE OMN2
C     NE IS THE NUMBER OF TOTAL ENERGIES AT WHICH THE PROGRAM IS RUN
C     NPST IS THE NUMBER OF PSEUDOSTATES
C
  100 FORMAT(5I5)
      CALL       OMN2(BBQ,CCQ,DDQ,LXN,TXN,ISKP,
     1     TKS,TKN,TNN,PPAS,BO,B1,XXS,YYS,EMTM,A,U,TM,AX,AO,A1,RO
     2,ROS,CD,SD,SMD,CMD,PMOO,PM11,PM10,PR,SCR,CSR,FR,CSX,LAT,LNN,KNX,K2
     3,KNLM,NMMAX,N2,KNMAX,NCHMX,NWRT,NPUN,NE,ICSWT,IOMN,NPST,KPUN)
      STOP
      END
```

```
      SUBROUTINE MPT1K(BFAS,BFAT,FFAS,FFAT,TKS,LCH,LAT,KAT,NCHMX,
     1                 NCAT,NBIG,NDMX)
C*****************************************************************
C     BASIC SUBROUTINE FOR E-HYDROGENLIKE  IONS SCATTERING
C     GENERATES BOUND-BOUND,BOUND-FREE,AND FREE-FREE MATRIX ELEMENTS
C     NECESSARY FOR THE EVALUATION OF K-MATRIX ELEMENTS IN THE
C     FRAMEWORK OF A CLOSE-COUPLING CALCULATION ,USING THE 'ALGEBRAIC
C     VARIATIONAL METHOD' ..........................................
C      PARITY=(-1)**L
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION BFD(10,2),BFX(10,2),FFD(2,2),FFX(2,2),BND(10,10),BNX(10,
     110),SD(10,10),SX(10,10)
      DIMENSION FC(11) ,GC(11),FCP(11),GCP(11)
      DIMENSION LCH(NCHMX),TKS(NCHMX),LAT(NCHMX),KAT(NCHMX)
      DIMENSION CEIG(5,10,10),NPWR(5,10),ENEG(5,10),          WT(5,10),
     1Z(5,10),ZSC(10,50),NSC(10,50),ZETA(50),P(1200)
     2 , NSTL(5),NOSAZ(5)
      DIMENSION BFAS(NBIG,NCAT,2),BFAT(NBIG,NCAT,2)
      DIMENSION FFAS(NCAT,2,NCAT,2),FFAT(NCAT,2,NCAT,2)
      DIMENSION FPK(1200,11),GPK(1200,11),DFPK(1200,11),DGPK(1200,11)
      LOGICAL IRED,JPUN,JWRT,ITAPE,IDISK
C
C     ..............LOGICAL VARIABLES.............................
C
C     IF IRED=FALSE,FF. MATRICES ARE COMPUTED & WRITTEN ON DISK
C     IF IRED=TRUE,FF. MATRICES ARE READ FROM DISK AND NEWLY COMPUTED
C       FF. ELEMENTS ARE WRITTEN ON DISK
C      IF JWRT=TRUE, FFD-X  VALUES ARE WRITTEN
C      IF ITAPE=TRUE,TAPE CONTAINING SINGLET & TRIPLET MATRICES
C      IS WRITTEN
C     IF IDISK=TRUE,BB. & BF. MATRICES ARE NOT COMPUTED
C     ..............................................................
C
C     ........................COMMON BLOCKS.........................
C     COMMON/ABC PASSES CHANNEL PARAMETERS
C     COMMON/FFR PASSES COULOMB FUNCTIONS & THEIR FIRST DERIVATIVES
C                TO FREE-FREE FUNCTIONS AND SUBROUTINES
C     COMMON/BFR PASSES COULOMB FUNCTIONS TO BOUND-FREE FUNCTIONS &
C                SUBROUTINES
C     COMMON/BODE PASSES NUMERIC INTEGRATION PARAMETERS
C     ..............................................................
C
      COMMON/ABC/GAM,EN,CEIG,Z,P,Q,BAR,   C,ENEG,L,LZ,LQ,LA,LP,NBSA,NBSZ
     1,NPWR,L2,  L1 ,KB,JC,NA,NZ,NMAX ,NZCH
      COMMON/BODE/DELR,R,NPTS
      COMMON/FFR/FP(1200),GP(1200),DFP(1200),DGP(1200),FQ(1200),GQ(1200)
      COMMON/BFR/FPC(1200),GPC(1200)
      WRITE(6,881)
  881 FORMAT(1X,'MAX. # OF CHANNELS',2X,'MAX. # OF OPEN CHANNELS',2X,'MA
     1X. DIMENSION OF BOUND-BOUND MATRIX',2X,'MAX. DIMENSION OF PSEUDOPA
     2SIS',1X/)
      WRITE(6,999)
      WRITE(6,1234)NCHMX,NCAT,NBIG,NDMX
 1234 FORMAT(5X,I5,15X,I5,23X,I5,35X,I5)
      ACCUR=1.D-12
      STEP=999.D0
      NMAX=NDMX
      READ(5,114)IRED,JPUN,JWRT,ITAPE,IDISK
  114 FORMAT(5L5)
```

```
      ICHXX=0
      JCHXX=0
      L1XX=0
      L2XX=0
      IF(.NOT.IRED) GO TO 1239
      DO 1235 I=1,99999
      READ(9,397,END=1236)ICHXX,JCHXX,L1XX,L2XX,FFD,FFX
 1235 CONTINUE
 1236 CONTINUE
      WRITE(6,882)
  882 FORMAT(1X,'CHANNEL INDICES OF THE LAST FF. ELEMENT(CALCULATED &
     1STORED ON DISC;UNIT 9) ',1X/)
      WRITE(6,106)ICHXX,JCHXX,L1XX,L2XX
  106 FORMAT(10I5)
 1239 READ(5,100)L
C     ..........L IS THE TOTAL ANGULAR MOMENTUM OF THE SYSTEM.........
      REWIND 9
  100 FORMAT(I5)
      IBF=0
      IFF=0
      READ(5,100) NZCH
C     ............NZCH IS THE NUCLEAR CHARGE OF THE ION................
      ZCH=DFLOAT(NZCH)
      DZ3=DSQRT(ZCH**3)
      READ(5,103) RMN
      READ(5,103) RMX
      READ(5,100) NPTS
C
C     ................NUMERIC INTEGRATION PARAMETRS..................
C     RMN AND RMX ARE RESPETIVELY THE MIN. AND MAX. RADIAL DISTANCES
C     USED IN THE NUMERIC INTEGRATION.NPTS IS THE NUMBER OF POINTS
C     IN THAT REGION.DELR IS THE MESH SIZE.........................
C     ............................................................
C
      DELR=(RMX-RMN)/DFLOAT(NPTS-1)
      R(1)=RMN
      DO 1011 I=2,NPTS
 1011 R(I)=R(I-1)+DELR
  103 FORMAT(F10.5)
C
C     ..............CHANNEL PARAMETERS.........................
C
      READ(5,100)NATL
C     NATL= NUMBER OF IONIC  L VALUES
C
      READ(5,100) (NBSAZ(I),I=1,NATL)
C     NBSAZ IS THE NUMBER OF PSEUDO STATES FOR ANGULAR MOMENTUM L IONIC
C
      IKWD=1
      IKWX=2
      NL=NATL+L-1
      NL1=NL+1
      DO 1 I=1,NATL
      NBSZ=NBSAZ(I)
      DO 1 J=1,NBSZ
      READ(5,101)NT(I,J),NNN,ENEG(I,J)
    1 ENEG(I,J)=ENEG(I,J)*ZCH**2
  101 FORMAT(2I5,D25.14)
C
C     NT(I,J) REPRESENTS THE # OF TERMS IN J-TH PSEUDOSTATE OF ANGULAR
```

```
C     MOMENTUM I.ENEG(I,J) IS THE ENERGY OF THAT PARTICULAR TERM.....
C     WHN IS EQUAL TO ANGULAR MOMENTUM OF THE TARGET STATE.....
C
      DO 1000 I=1,NATL
      NBSZ=NBSAZ(I)
       READ(5,102)  (NPWR(I,J),Z(I,J),J=1,NBSZ)
 1000 CONTINUE
  102 FORMAT(I5,F19.14)
C
C     NPWR AND Z ARE RESPECTIVELY THE POWERS  AND EXPONENTS  OF THE
C     OF THE PSEUDOBASIS.CEIG REPRESENT THE COEFFICIENTS WHICH MULTIPLY
C     THE PSEUDOBASIS ELEMENTS IN THE EXPANSION OF A PARTICULAR TARGET
C     STATE.....
C
      DO 2 I=1,NATL
      NBSZ=NBSAZ(I)
      DO 2 J=1,NBSZ
      K=NT(I,J)
      Z(I,J)=Z(I,J)*ZCH
      DO 2 M=1,NBSZ
      CEIG(I,J,M)=0.0
      IF(M.GT.K) GO TO 2
      READ(5,104) CEIG(I,J,M)
      CEIG(I,J,M)=CEIG(I,J,M)*DZ3*ZCH**NPWR(I,M)
  104 FORMAT(24X,F19.14)
    2 CONTINUE
      READ(5,100)ILLI
C
C     ILLI GE. 0 DECIDES THE SHAPE OF THE SHORT RANGE BASIS USED IN
C     THE EXPANSION OF THE SCATTERING FUNCTION
C
      IF(ILLI.GT.0)GO TO 3
      READ(5,100)NSTO
      READ(5,103) (ZETA(I),I=1, NSTO)
C     ..................SHORT RANGE BASIS.............................
C      NSTO IS THE # OF SLATER-TYPE ORBITALS USED IN THE SHORT RANGE
C      BASIS.ZETA(I)  IS THE EXPONENT OF THE I-TH SLATER ORBITAL.......
C     ..............................................................
      GO TO 5
    3 READ(5,100)NSCL
      DO 4 I=1,NSCL
      READ(5,100)NSTL(I)
C
C     NSCL=NUMBER OF SCATTERING ANGULAR MOMENTA, NSCL = NL1
C     NSTL(I) =NUMBER OF SHORT RANGE NESBET FUNCTIONS FOR ANG. MOM. I
C
      K=NSTL(I)
    4 READ(5,105) (NSC(I,J),ZSC(I,J),J=1,K)
  105 FORMAT(I5,F10.5)
C     ....REDEFINING THE COEFFICIENTS OF THE 1S,2S AND 2P STATES.....
    5 CEIG(1,1,1)=2.D0*DZ3
      CEIG(1,2,2)=0.5D0*DSQRT(2.D0)*DZ3
      CEIG(1,2,3)=-0.5D0*ZCH*CEIG(1,2,2)
      CEIG(2,1,2)=ZCH*DZ3/(2.D0*DSQRT(6.D0))
      READ(5,103)EN
C
C     ....EN IS THE TOTAL ENERGY OF THE ELECTRON-ION SYSTEM.....
      READ(5,103)GAM
C
C     ...THE PARAMETER GAMMA WHICH APPEARS IN THE REGULARIZING FACTOR OF
```

```
C     IRREGULAR COULOMB FUNCTION.....................................
C
      ICH=0
      NCH=0
      NDIF=0
      NDIB=0
C
C     CHANNEL ANALYSIS :
C
      DO 700 I=1,NATL
      NBSZ=NBSAZ(I)
      LX=I-L-1
      LX=IABS(LX)
      LY=I+L-1
      NRAN=1+(1+LY-LX)/2
      DO 7 K=1,NBSZ
      TK=EN-ENEG(I,K)
      LL=LX
      DO 6 J=1,NRAN
      ICH=ICH+1
      LCH(ICH)=LL
      IF(TK.GE.0.0) NCH=NCH+1
      IF(TK.GE.0.0) TKS(ICH)=DSQRT(TK)
      IF(TK.LT.0.0D0) TKS(ICH)=-DSQRT(DABS(TK))
      LAT(ICH)=I-1
      LLX=LL+1
      KAT(ICH)=K
      IF(ILLI.EQ.0) NSTQ=NSTO
      IF(ILLI.GT.0) NSTQ=NSTL(LLX)
      NDIB=NDIB+NSTQ
      IF(TK.GT.0.0.AND.ICH.GT.1)                    NDIF=0
      LL=LL+2
      IF(LL.GT.LY) GO TO 7
    6 CONTINUE
    7 CONTINUE
  700 CONTINUE
      NCHT=ICH
C
C     GENERATING THE COULOMB FUNCTIONS :
C
      DO 2222 KCH=1,NCHT
      IF(TKS(KCH).LT.0.0) GO TO 2222
      PK=TKS(KCH)
      LK=LCH(KCH)
      ETAP=-(ZCH-1.D0)/PK
      DO 2222 IK=1,NPTS
      RHO=PK*R(IK)
      CALL RCWFN(RHO,ETAP,LK,LK,FC,FCP,GC,GCP,ACCUR,STEP)
      FPK(IK,KCH)=FC(LK+1)
      GPK(IK,KCH)=GC(LK+1)
      DFPK(IK,KCH)=FCP(LK+1)*PK
      DGPK(IK,KCH)=GCP(LK+1)*PK
 2222 CONTINUE
      NDIM=NDIB+NDIF
      WRITE(6,883) ZCH
  883 FORMAT(1X,'NUCLEAR CHARGE=',F10.5,1X/)
      RMN=0.0001D0
      WRITE(6,884) RMX
  884 FORMAT(1X,'R MAX.=',F10.5,1X/)
      WRITE(6,885) DELR
```

```
  885 FORMAT(1X,'MESH SIZE=',F10.5,1X/)
      WRITE(6,886)   NPTS
  886 FORMAT(1X,'NUMBER OF MESHES=',I5,1X/)
      WRITE(6,887)NCHT
  887 FORMAT(1X,'ACTUAL MAX. # OF CHANNELS=',I5,1X/)
      WRITE(6,888)NCH
  888 FORMAT(1X,'ACTUAL # OF OPEN CHANNELS=',I5,1X/)
      WRITE(6,889)NDIB
  889 FORMAT(1X,'ACTUAL DIMENSION OF THE BB. MATRIX=',I8,1X/)
      WRITE(6,991)NDIM
  991 FORMAT(1X,'CORRECTED DIMENSION OF BB. MATRIX=',I5,1X/)
      LMX=NDIM*(NDIM+1)/2
      WRITE(6,115)LMX
  115 FORMAT(1X,'LMX=NDIM*(NDIM+1)/2=',I8,1X/)
      WRITE(6,993)
  993 FORMAT(5X,'PSEUDOSTATE ANG. MOM.',2X,'# OF PSEUDOSTATES FOR A SPEC
     1IFIC L',5X,'CHANNEL ANG MOM',12X,'CHANNEL ENERGY(IN RY)',1X/)
      DO 511 I=1,NCHT
      TK=TKS(I)*TKS(I)
      IF(TKS(I).LT.0.0)TK=0.0
  511 WRITE(6,113)I,LAT(I),KAT(I),LCH(I),TK
  113 FORMAT(I4,10X,I5,28X,I5,20X,I5,22X,F10.5)
      WRITE(6,105)
      DO 1008 IAX=1,NDIM
      DO 1008 JAJ=1,NCH
      DO 1008 IA=1,2
      BPAS(IAX,JAJ,IA)=0.0
 1008 BPAT(IAX,JAJ,IA)=0.0
      DO 1009 IAX=1,NCH
      DO 1009 JAJ=1,NCH
      DO 1009 IA=1,2
      DO 1009 JB=1,2
      FPAS(IAX,IA,JAJ,JB)=0.0
 1009 FPAT(IAX,IA,JAJ,JB)=0.0
      NGGT=0
      TQQ=TKS(1)*TKS(1)
      IF(ILLI.EQ.0)WRITE(6,994)
      IF(ILLI.GT.0)WRITE(6,995)
      IF(ILLI.GT.0)GO TO 9
  994 FORMAT(1X,'SHORT RANGE BASIS EXPONENTS(ZETA)',1X//)
      WRITE(6,206)(I,ZETA(I),I=1,NSTO)
  206 FORMAT(I5,D24.14)
      GO TO 11
  995 FORMAT(1X,'SHORT RANGE BASIS EXPONENTS FOR A PARTICULAR TARGET
     1ANGULAR MOMENTUM',1X/)
    9 DO 10 I=1,NSCL
      NSTQ=NSTL(I)
      DO 10 J=1,NSTQ
      WRITE(6,111)I,J,NSC(I,J),ZSC(I,J)
  111 FORMAT(3I5,D26.14)
  202 FORMAT(1H )
   10 CONTINUE
   11 WRITE(6,202)
      ICNTR=0
      WRITE(6,996)
  996 FORMAT(1X,'TOTAL ENERGY',2X,'GAMMA',2X,'INCIDENT ENERGY',1X/)
      WRITE(6,205)EN,GAM,TQQ
  205 FORMAT(3F11.6)
      WRITE(6,999)
  999 FORMAT(1H1)
```

```
      DO 12 I=1,NL1
      IF(ILLI.EQ.0) NSTQ=NSTO
      IF(ILLI.GT.0) NSTQ=NSTL(I)
   12 CONTINUE
      NIDX=0
C
C     GENERATING AND STORING THE BOUND-BOUND MATRIX ELEMENTS :
C
      DO 311JZ=1,NATL
      NBSZ=NBSAZ(JZ)
      LZ=JZ-1
      LX=LZ-L
      LX=IABS(LX)
      LY=LZ+L
      NRAN=1+(1+LY-LX)/2
      LQ=LX
      DO 310ILS=1,NRAN
      NGGT=NGGT+1
      JQ=LQ+1
      IF(ILLI.EQ.0) NNN=NSTO
      IF(ILLI.GT.0) NNN=NSTL(JQ)
      DO 31 IU=1,NNN
      IF(ILLI.GT.0) GO TO 13
      BAB=ZETA(IU)
      KB=LQ
      GO TO 14
   13 KB=NSC(JQ,IU)
      BAB=ZSC(JQ,IU)
   14 N1=NIDX+IU
      NJDX=0
      N5=NDIB
      DO 221 JA=1,NATL
      NBSA=NBSAZ(JA)
      LA=JA-1
      LXA=LA-L
      LXA=IABS(LXA)
      LYA=LA+L
      NRAN=1+(1+LYA-LXA)/2
      LP=LXA
      DO 22 JLS=1,NRAN
      JP=LP+1
      IF(ILLI.EQ.0) MMM=NSTO
      IF(ILLI.GT.0) MMM=NSTL(JP)
      DO 21 JV=1,MMM
      IF(ILLI.GT.0) GO TO 16
      C=ZETA(JV)
      JC=LP
      GO TO 17
   16 JC=NSC(JP,JV)
      C=ZSC(JP,JV)
   17 CONTINUE
   18 N2=NJDX+JV
      IF(N2.LT.N1) GO TO 21
      IF(.NOT.IDISK)  CALL CBNMX(BND,BNX,SD,SX)
      N3=N1
      DO 20 NA=1,NBSZ
      N4=N2
      DO 19 NB=1,NBSA
      IF(N3.LE.N4) K34=N3+(N4*(N4-1))/2
      IF(N3.GT.N4) K34=N4+(N3*(N3-1))/2
```

```
      B           = BND(NA,NB)+BNX(NA,NB)
      EMAT        = BND(NA,NB)-BNX(NA,NB)
      WRITE(1)K34,B,EMAT
      IF(ITAPE)WRITE(3,115)K34,B,EMAT
      ICNTR=ICNTR+1
   19 N4=N4+MMM
   20 N3=N3+NNN
   21 CONTINUE
      LP=LP+2
      NJDX=NJDX+MMM*NBSA
      IF(LP.GT.LYA)GO TO 222
   22 CONTINUE
  222 CONTINUE
  221 CONTINUE
      JOCH=0
C
C     GENERATING AND STORING THE BOUND-FREE MATRIX ELEMENTS :
C
      DO 30 JCH=1,KCHT
      IF(TKS(JCH).LT.0.0)GO TO 30
      P=TKS(JCH)
      LA=LAT(JCH)
      LP=LCH(JCH)
      NA=KAT(JCH)
      DO 1012 IPH=1,NPTS
      FPC(IPH)=FPK(IPH,JCH)
 1012 GPC(IPH)=GPK(IPH,JCH)
      JA=LA+1
      NBSA=NBSAZ(JA)
      JOCH=JOCH+1
      LLL=  1
      DO 29 L2=1,LLL
      IF(.NOT.IDISK) CALL CBFMX(BFD,BFX,SD,SX)
      DO 24 IIA=1,2
      N3=N1
      DO 23 NQ=1,NBSZ
      BQX= BFD(NQ,IIA)-BFX(NQ,IIA)
      BQD= BFD(NQ,IIA)+BFX(NQ,IIA)
      BFAS(N3,JOCH,IIA)=BFAS(N3,JOCH,IIA)+BQD
      BFAT(N3,JOCH,IIA)=BFAT(N3,JOCH,IIA)+BQX
      WRITE(2)N3,JOCH,IIA,BFAS(N3,JOCH,IIA),BFAT(N3,JOCH,IIA)
      IBF=IBF+1
   23 N3=N3+NNN
   24 CONTINUE
   29 CONTINUE
   30 CONTINUE
   31 CONTINUE
      LQ=LQ+2
      NIDX=NIDX+NBSZ*NNN
      IF(LQ.GT.LY)GO TO 312
  310 CONTINUE
  312 CONTINUE
  311 CONTINUE
      N5=NDIB
      IOCH=0
C
C     GENERATING AND STORING THE FREE-FREE MATRIX ELEMENTS :
C
      WRITE(6,999)
      IF(JWRT)WRITE(6,997)
```

```
  997 FORMAT(1X,'CALCULATED AND STORED FF. MATRIX ELEMENTS : ',1X//)
      DO 44 ICH=1,KCHT
      Q=TKS(ICH)
      IF(Q.LT.0.0)GO TO 44
      LZ=LAT(ICH)
      LQ=LCH(ICH)
      NZ=KAT(ICH)
      DO 4444 IQ=1,NPTS
      FQ(IQ)=FPK(IQ,ICH)
 4444 GQ(IQ)=GPK(IQ,ICH)
      JZ=LZ+1
      NBSZ=NBSAZ(JZ)
      IOCH=IOCH+1
      LLK=    1
      DO 43 L1=1,LLK
      N6=N5
      JOCH=IOCH-1
      DO 422 JCH=ICH,KCHT
      P=TKS(JCH)
      IF(P.LT.0.0)GO TO 422
      JOCH=JOCH+1
      IF(JOCH.GT.NCH) GO TO 423
      LA=LAT(JCH)
      LP=LCH(JCH)
      DO 5555 IP=1,NPTS
      FP(IP)=FPK(IP,JCH)
      GP(IP)=GPK(IP,JCH)
      DFP(IP)=DFPK(IP,JCH)
 5555 DGP(IP)=DGPK(IP,JCH)
      NA=KAT(JCH)
      JA=LA+1
      NBSA=NBSAZ(JA)
      LLL=    1
      DO 42 L2=1,LLL
      IF( .NOT.IRED)CALL CFFMX(FFD,FFX,SD,SX)
      IF(.NOT.IRED)GO TO 3959
      READ(9,397)ITA,ITB,ITC,ITD,FFD,FFX
  397 FORMAT(4A4,4A8,4A8)
      IF(ITD.EQ.L2.AND.ITC.EQ.L1.AND.ITB.EQ.JCH.AND.ITA.EQ.ICH)GO TO 396
      WRITE(6,398)ITA,ITB,ITC,ITD,ICH,JCH,L1,L2
  398 FORMAT(4I5,5X,4I5)
 3959 IF(JPUN)WRITE(7,397)ICH,JCH,L1,L2,FFD,FFX
      WRITE(9,397)ICH,JCH,L1,L2,FFD,FFX
 3958 FORMAT(5I5,4D25.14)
  396 IF(JWRT)WRITE(6,3958)ICH,L1,JCH,L2,IKWD,FFD
      IF(JWRT)WRITE(6,3958)ICH,L1,JCH,L2,IKWX,FFX
      DO 33 IIA=1,2
      DO 32 IJB=1,2
      FFAS(IOCH,IIA,JOCH,IJB)=FFAS(IOCH,IIA,JOCH,IJB)+FFD(IIA,IJB)
     1 +FFX(IIA,IJB)
      FFAT(IOCH,IIA,JOCH,IJB)=FFAT(IOCH,IIA,JOCH,IJB)+FFD(IIA,IJB)-
     1 FFX(IIA,IJB)
      WRITE(4)IOCH,IIA,JOCH,IJB,FFAS(IOCH,IIA,JOCH,IJB),FFAT(IOCH,IIA,
     1JOCH,IJB)
      IFF=IFF+1
   32 CONTINUE
   33 CONTINUE
   41 CONTINUE
      IF(ICH.LT.ICHXX)GO TO 42
      IF(ICH.EQ.ICHXX.AND.L1.LT.L1XX)GO TO 42
```

```
      IF(ICH.EQ.ICHXX.AND.L1.EQ.L1XX.AND.JCH.LT.JCHXX)GO TO 42
      IF(ICH.EQ.ICHXX.AND.L1.EQ.L1XX.AND.JCH.EQ.JCHXX.
     1   AND.L2.LT.L2XX)GO TO 42
      IRED=.FALSE.
   42 CONTINUE
      IF(L1.NE.LLK) GO TO 422
      IF(IOCH.EQ.JOCH)GO TO 422
      DO 421 IIA=1,2
      DO 421 IJB=1,2
      FFAS(JOCH,IJB,IOCH,IIA)=FFAS(IOCH,IIA,JOCH,IJB)
      FFAT(JOCH,IJB,IOCH,IIA)=FFAT(IOCH,IIA,JOCH,IJB)
      WRITE(4)JOCH,IJB,IOCH,IIA,FFAS(JOCH,IJB,IOCH,IIA),FFAT(JOCH,IJB,
     1IOCH,IIA)
      IFF=IFF+1
  421 CONTINUE
  422 CONTINUE
  423 CONTINUE
      IF(LLK.GE.2.AND.L1.EQ.LLK.AND.Q.GT.1.0D-08.AND.ICH.GT.1) N5=N5+2
   43 CONTINUE
   44 CONTINUE
   50 CONTINUE
      WRITE(6,105)
      WRITE(6,998)
  998 FORMAT(1X,'COUNTERS FOR BB.,BF.,AND FF. ELEMENTS :',1X/)
      WRITE (6,3957)ICNTR,IBF,IFF
 3957 FORMAT(3I8)
C
C     STORING CHANNEL PARAMETERS
C
      WRITE(8)ICNTR,IBF,IFF,NCH,KCHT,LMX,L,NDIM
      WRITE(8)(TKS(I),I=1,KCHT)
      WRITE(8)(LAT(I),I=1,KCHT)
      RETURN
      END
```

```
      SUBROUTINE MPT2C(BPAS,BPAT,FFAS,FFAT,B,D,TKS,MGMM,MGND,MBIG,MCAT,
     1MCHMX)
C*****************************************************************************
C     WRITTEN BY DR J. CALLAWAY.REVISED BY DR L. MORGAN. FINAL REVISION
C     BY N. ABU-SALBI
C     INVERTS BOUND-BOUND MATRIX AND CONSTRUCTS THE VARIATIONAL M-
C     MATRIX
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION TKS(MCHMX)
      DIMENSION FFAS(MCAT,2,MCAT,2),FFAT(MCAT,2,MCAT,2)
      DIMENSION BPAS(MBIG,MCAT,2),BPAT(MBIG,MCAT,2)
      DIMENSION B(MGMM),D(MGND)
      INTEGER D
      REAL*16 Q
C
C     READS IN CHANNEL PARAMETERS
C
      READ(8)ICNTR,IBF,IFF,MCH,KCHT,LMX,L,MDIM
      READ(8)(TKS(I),I=1,KCHT)
      REWIND 8
C
C     READS IN BOUND-FREE,FREE-FREE,& BOUND-BOUND MATRIX ELEMENTS
C
      DO 1 IX=1,IBF
      READ(2)M,ICH,IIA,BPAS(M,ICH,IIA),BPAT(M,ICH,IIA)
 1    CONTINUE
      REWIND 2
      DO 9 IX=1,IFF
 9    READ(9)IA,IB,IC,ID,FFAS(IA,IB,IC,ID),FFAT(IA,IB,IC,ID)
      REWIND 9
      IFF=0
C     BEGIN SPIN LOOP
      DO 80 IAS=1,2
C     INVERTS BOUND-BOUND MATRIX
      DO 3 I=1,ICNTR
      READ(1) K,QA,QB
      IF (IAS.EQ.1) QC=QA
      IF (IAS.EQ.2) QC=QB
 3    B(K)=      (QC)
C
C     REPLACES B WITH ITS (UPPER) TRIANGULAR FACTORIZATION
C
      DO 610 I=1,NDIM
      II=I*(I-1)/2
      KII=I+II
      DO 609 J=I,NDIM
      JJ=J*(J-1)/2
      KIJ=I+JJ
      Q=0.0Q0
      IF(I.EQ.1) GO TO 605
      MM=I-1
      KNI=II
      KNJ=JJ
      DO 604 NU=1,MM
      KNI=KNI+1
      KNJ=KNJ+1
      IF(D(NU).GT.0) GO TO 603
      Q=Q+B(KNI)*B(KNJ)
      GO TO 604
```

```
 603  Q= Q-B(KMI)*B(KMJ)
 604  CONTINUE
  605 Q=QEXTD(B(KIJ))+Q
      IF(I.EQ.J) GO TO 608
      IF(D(I).GT.0) GO TO 607
      B(KIJ)=-Q/B(KII)
      GO TO 609
 607  B(KIJ)=Q/B(KII)
      GO TO 609
 608  D(I)=1
      IF(Q.LT.0.000)  D(I)=-1
      Q=QABS(Q)
      B(KII)=QSQRT(Q)
 609  CONTINUE
 610  CONTINUE
C
C     COUNTS SINGLET (OR TRIPLET) IGENVALUES
C
      NRES=0
      DO 2 I=1,NDIM
      IF(D(I).LT.0)  NRES=NRES+1
  2   CONTINUE
      IF(IAS.EQ.1) PRINT 4,NRES
      IF(IAS.EQ.2) PRINT 5,NRES
  4   FORMAT(/'  SINGLET EIGENVALUES COUNT',I5)
  5   FORMAT(/'  TRIPLET EIGENVALUES COUNT',I5)
C
C     CONSTRUCTS AND STORES H-MATRIX ELEMENTS
C
      DO 664 ICH=1,NCH
      DO 664 IIA=1,2
      DO 664 I=1,NDIM
      Q=QEXTD(BPAS(I,ICH,IIA)    )
      I1=I-1
      I2=I*I1/2
      KII=I+I2
      IF(I.EQ.1) GO TO 664
      DO 663 K=1,I1
      KIJ=K+I2
 663  Q= Q-B(KIJ)*     (BPAS(K,ICH,IIA))
  664 BPAS(I,ICH,IIA)=Q/B(KII)
 619  CONTINUE
      DO 622 ICH=1,NCH
      DO 622 IIA=1,2
      DO 622 JCH=1,NCH
      DO 622 JJA=1,2
      KKA=IIA+2*(JJA-1)+4*(IAS-1)
      Q= QEXTD(FPAS(ICH,IIA,JCH,JJA))
      DO 620 K=1,NDIM
      IF(D(K).GT.0) GO TO 621
      Q= Q+     (BPAS(K,ICH,IIA))*     (BPAS(K,JCH,JJA))
      GO TO 620
 621  Q= Q-     (BPAS(K,ICH,IIA))*     (BPAS(K,JCH,JJA))
 620  CONTINUE
      FPAS(ICH,IIA,JCH,JJA)=Q
      WRITE(4) ICH,IIA,JCH,JJA,Q
 622  CONTINUE
 650  CONTINUE
      REWIND 1
      IF(IAS.EQ.2) GO TO 80
```

```
      DO 77 I=1,NDIM
      DO 77 J=1,NCH
      DO 77 IIA=1,2
 77   BFAS(I,J,IIA)=BFAT(I,J,IIA)
      DO 79 I=1,NCH
      DO 79 J=1,NCH
      DO 79 IIA=1,2
      DO 79 IJA=1,2
 79   FFAS(I,IIA,J,IJA)= FFAT(I,IIA,J,IJA)
 80   CONTINUE
C
C     END OF SPIN LOOP
C
      REWIND 1
      RETURN
      END
```

```
      SUBROUTINE NORM(L,ETA,XN)
C*****************************************************************
C     GENERATES REGULAR COULOMB FUNCTION NORMALIZATION(XN) FOR ALL
C     ANGULAR MOMENTA(L) AND PARAMETRS(ETA)
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      PI=3.1415926535897900
      PIE=2.D0*PI*ETA
      C1=PIE/(DEXP(PIE)-1.D0)
      C1=DSQRT(C1)
      IF(L.NE.0) GO TO 1
      XN=C1
      RETURN
    1 DL=DFLOAT(L)
      DO  10 I=1,L
      DI=DFLOAT(I)
      DII=DI*(2.D0*DI+1.D0)
      DIE=DI*DI+ETA*ETA
      CL=DSQRT(DIE)*C1/DII
      C1=CL
   10 CONTINUE
      XN=CL
      RETURN
      END
```

```
      SUBROUTINE OMN2(BBQ,CCQ,DDQ,LXN,TXN,ISKP,
     1     TXS,TXR,TNN,PPAS,BO,B1,EES,TTS,EMTA,A,U,TR,AE,AO,A1,RO
     2,ROS,CD,SD,SRD,CRD,PROO,PR11,PR10,PR,SCR,CSR,PR,CSE,LAT,LNN,KNI,K2
     3,KNLM,NMMAX,N2,KMMAX,NCMAX,MUNT,NPUN,NE,ICSNT,IOMN,NPST,KPUN)
C**********************************************************************
C     WRITTEN BY DR J. CALLAWAY. REVISED FEB. 1981
C    COMPUTES REACTANCE (OR K-) MATRIX ELEMENTS ON THE THE BASIS OF THE
C    'ALGEBRAIC VARIATIONAL METHOD' USING OMN & IOMN FORMULAS
C**********************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION TXS(NCMAX),LAT(NCMAX),TXN(NCMAX),TNN(NCMAX),LNN(NCMAX)
      DIMENSION PPAS(KNI,2,KNI,2),BO(KNI,KNI),B1(KNI,KNI),EES(KNI,KNI),
     1TTS(KNI,KNI),EMTA(NMMAX),A(KNLM,KNLM),U(KNLM,KNLM),TR(KNLM,KNLM),
     2AE(N2),AO(KNI,KNI),A1(KNI,KNI),ROS(KMMAX),          CD(KNI),SD
     3(KNI),SRD(KNI,KNI),CRD(KNI,KNI),PROO(KNI,KNI),PR11(KNI,KNI),PR10(K
     4NI,KNI),PR(KNI,KNI),SCR(KNI,KNI),CSR(K2),PR(KNI,KNI),CSI(KNI,KNI)
     5,RO(KNI,KNI),LXN(NCMAX),TXN(NCMAX)
      COMPLEX*16 BBQ(KNI,KNI),CCQ(KNI,KNI),DDQ(KNI)
      PI=3.1415926535898D0
C
C.....................CONTROL VARIABLES.....................
C     KNI = MAXIMUM DIMENSION OF (ORDINARY) MATRICES
C     ICSNT=NUMBER OF INITIAL CHANNELS FOR WHICH CROSS SECTIONS ARE
C      PRINTED. ICSNT MUST BE GE 1 AND LE NCH
C     IF IOMN=1,INVERSE OMN RESULTS WILL ALSO BE CALCULATED
C     IF MUNT GE. 1  CHANNEL ANGULAR MOMENTA AND ENERGIES ARE WRITTEN
C     IF MUNT GE. 2 R-MATRIX ELEMENTS ARE WRITTEN
C     NE IS THE NUMBER OF ENERGIES (USUALLY NE=1)
C     NPST IS THE NUMBER OF PSEUDOSTATES :3 FOR 3S-3P,0 FOR 6S-5P-2D-1F
C     IF KPUN=7 K-MATRICES ARE PUNCHED ON CARDS
C     IF KPUN=1 OMN AND IOMN K-MATRIX ELEMENTS ARE STORED ON UNITS
C     KPUN AND KPUN+1 RESPECTIVELY
C     IF ISKP GT. 0 SINGLET OR TRIPLET K-MATRIX ELEMENTS ARE NEITHER
C     STORED NOR PUNCHED  .
C
      NCAS=1
      IF(IOMN.EQ.1)NCAS=2
      K2=KNI*KNI
      N2=4*K2
      KMMAX=(KNI*(KNI+1))/2
      KPUN1=KPUN+1
      IF(KPUN.EQ.7)KPUN1=KPUN
      KNLM=2*KNI
      NMMAX=(KNLM*(KNLM+1))/2
      DO 2003 IER=1,NE
C
C     READS IN CHANNEL PARAMETERS :
C
      READ(8)IA,IB,IC,NCH,ID,IE,LT,JA
  901 FORMAT(3X,I5,15X,I5,15X,I5)
      WRITE(6,111)
  111 FORMAT(1X,'0 OF CHANNELS',2X,'TOTAL 0  OF CHANNELS',2X,'TOTAL ANGU
     1LAR MOMENTUM',1X//)
      WRITE(6,901)NCH,ID,LT
      NCNT=ID
      READ(8) (TNN(I),I=1,ID)
      WRITE(6,905)
      WRITE(6,223)
  223 FORMAT(1X,'CHANNEL ENERGIES',1X/)
      WRITE(6,905)
```

```
      IF(NWRT.GE.1)WRITE(6,903)(THN(I),I=1,ID)
  903 FORMAT(5X,F19.14)
      READ(8)(LNN(I),I=1,ID)
      WRITE(6,905)
      WRITE(6,333)
  333 FORMAT(1X,'ANGULAR MOMENTA OF PSEUDOSTATES :',1X/)
      IF(NWRT.GE.1)WRITE(6,902)(LNN(I),I=1,ID)
  902 FORMAT(19I4)
      J=0
      DO 750 I=1,ID
      LIN(I)=LNN(I)
      TIN(I)=THN(I)
      IF(THN(I).LT.0.0)GO TO 750
      J=J+1
      TKS(J)=THN(I)
      LAT(J)=LNN(I)
  750 CONTINUE
      TK2=TKS(1)*TKS(1)
      WRITE(6,905)
      WRITE(6,332)
  332 FORMAT(1X,'INCIDENT ENERGY',1X/)
      WRITE(6,908)TK2
      DO 1 I=1,NCH
    1 TKN(I)=DSQRT(TKS(I))
      DO 2002 IAS=1,2
      WRITE(6,905)
      IF(IAS.EQ.1)WRITE(6,444)
      IF(IAS.EQ.2)WRITE(6,555)
  444 FORMAT('    SINGLET',1X//)
  555 FORMAT('    TRIPLET',1X//)
      WRITE(6,905)
C
C     READS IN K-MATRIX ELEMENTS :
C
      DO 751 ICH=1,NCH
      DO 751 IIA=1,2
      DO 751 JCH=1,NCH
      DO 751 JJA=1,2
  751 READ(8)IA,IB,IC,ID,FFAS(IA,IB,IC,ID)
C
C     STARTS CALCULATING K-MATRIX ELEMENTS :
C
      DO 2 ICH=1,NCH
      DO 2 IIA=1,2
      IOCH=ICH+NCH*(IIA-1)
      DO 2 JCH=1,NCH
      DO 2 JJA=1,2
      JOCH=JCH+NCH*(JJA-1)
      A (IOCH,JOCH)=FFAS(ICH,IIA,JCH,JJA)/(TKN(ICH)*TKN(JCH))
    2 CONTINUE
  905 FORMAT(1H )
      NCH2=2*NCH
      DO 4 I=1,NCH2
      DO 4 J=I,NCH2
      KIJ=I+(J*(J-1))/2
      EATN(KIJ)=0.0
      DO 3 L=1,NCH2
    3 EATN(KIJ)=EATN(KIJ)+A(L,I)*A(L,J)
    4 CONTINUE
      CALL SIGEN(EATN,AI,NCH2,0,N2,NWMAI)
```

```
906 FORMAT(I5,F19.7)
  6 DO 7 I=1,NCH
    DO 7 J=1,NCH
    L=J+NCH
    M=I+NCH
    KIL=I+NCH2*(L-1)
    KML=M+NCH2*(L-1)
    A0(I,J)=AX(KIL)
    B0(I,J)=AX(KIL)
    B1(I,J)=AX(KML)
  7 A1(I,J)=AX(KML)
    DO 2001 ICAS=1,NCAS
    IF(ICAS.EQ.1) WRITE(6,666)
    IF(ICAS.EQ.2) WRITE(6,777)
666 FORMAT(1X,'OMN RESULTS',1X//)
777 FORMAT(1X,'IOMN RESULTS',1X//)
    CALL GMIS(NCH,A0,B0,CD,DET,KMX)
    DO 9 I=1,NCH
    DO 9 J=1,NCH
    R0(I,J)=0.0
    DO 8 K=1,NCH
  8 R0(I,J)=R0(I,J)+A1(I,K)*A0(K,J)
  9 CONTINUE
    DO 10 I=1,NCH
    DO 10 J=I,NCH
    KIJ=I+(J*(J-1))/2
 10 ROS(KIJ)=0.500*(R0(I,J)+R0(J,I))
    CALL SIGEN(ROS,CSR,NCH,0,K2,KMMAX)
    DO 11 I=1,NCH
    KII=I+(I*(I-1))/2
    QP=ROS(KII)*ROS(KII)+1.0
    QP=DSQRT(QP)
    IF(ICAS.EQ.2)GO TO 711
    CD(I)=1.00/QP
    SD(I)=ROS(KII)/QP
    GO TO 11
711 CD(I)=ROS(KII)/QP
    SD(I)=1.00/QP
 11 CONTINUE
    DO 13 I=1,NCH
    DO 13 J=1,NCH
    CMD(I,J)=0.0
    SMD(I,J)=0.0
    DO 12 K=1,NCH
    KIK=I+(K-1)*NCH
    KJK=J+(K-1)*NCH
    CMD(I,J)=CMD(I,J)+CSR(KIK)*CD(K)*CSR(KJK)
 12 SMD(I,J)=SMD(I,J)+CSR(KIK)*SD(K)*CSR(KJK)
    U(I,J)=CMD(I,J)
    K=I+NCH
    L=J+NCH
    U(K,J)= SMD(I,J)
    U(I,L)=-SMD(I,J)
 13 U(K,L)= CMD(I,J)
    DO 15 I=1,NCH2
    DO 15 J=1,NCH2
    TM(I,J)=0.0
    DO 14 K=1,NCH2
    DO 14 L=1,NCH2
 14 TM(I,J)=TM(I,J)+U(F,I)*A  (K,L)*U(L,J)
```

```
   15 CONTINUE
      DO 16 I=1,NCH
      DO 16 J=1,NCH
      PH00(I,J)=PR(I,J)
      K=I+NCH
      L=J+NCH
      IF(ICAS.EQ.2)GO TO 715
      PH10(I,J)=PR(K,J)
      GO TO 16
  715 PH10(I,J)=PR(J,K)
   16 PH11(I,J)=PR(K,L)
      IF(ICAS.EQ.1)  CALL GAIS(NCH,PH11,A1,CD,DET,KKK)
      IF(ICAS.EQ.2)  CALL GAIS(NCH,PH00,A1,CD,DET,KKK)
      WRITE(6,888)
  888 FORMAT(1X,'DET(H)  =',1X/)
      WRITE(6,908)DET
  908 FORMAT(E19.7)
      WRITE(6,905)
      DO 18 I=1,NCH
      DO 18 J=1,NCH
      QQ=0.0
      DO 17 K=1,NCH
      DO 17 L=1,NCH
      IF(ICAS.EQ.2)GO TO 716
      QQ=QQ           +PH10(K,I)*PH11(K,L)*PH10(L,J)
      GO TO 17
  716 QQ=QQ           -PH10(K,I)*PH00(K,L)*PH10(L,J)
   17 CONTINUE
      IF(ICAS.EQ.2)GO TO 717
      PR(I,J)=QQ-PH00(I,J)
      GO TO 18
  717 PR(I,J)=QQ+PH11(I,J)
   18 CONTINUE
      IF(ICAS.EQ.2)CALL GAIS(NCH,PR,A1,CD,DET,KKK)
      DO 20 I=1,NCH
      DO 20 J=1,NCH
      CSR(I,J)=CRD(I,J)
      SCR(I,J)=SRD(I,J)
      DO 19 K=1,NCH
      SCR(I,J)=SCR(I,J)+CRD(I,K)*PR(K,J)
   19 CSR(I,J)=CSR(I,J)-SRD(I,K)*PR(K,J)
   20 CONTINUE
      CALL GAIS(NCH, CSR,A1,CD,DET,KKK)
      DO 22I=1,NCH
      DO 22J=1,NCH
      PR(I,J)=0.0
      DO 21 K=1,NCH
   21 PR(I,J)=PR(I,J)+SCR(I,K)*CSR(K,J)
   22 A1(I,J)=0.0
      IF(ISKP.EQ.1.AND.IAS.EQ.2)GO TO 1109
      IF(ISKP.EQ.2.AND.IAS.EQ.1)GO TO 1109
      IF(ICAS.EQ.1.AND.KPUN.GT.0)WRITE(KPUN,911)TK2
      IF(ICAS.EQ.2.AND.KPUN.GT.0)WRITE(KPUN1,911)TK2
 1109 CONTINUE
C
C     STORES R-MATRICES:                    :
C
      WRITE(6,999)
  999 FORMAT(28X,'R MATRIX',1X,//)
      DO 221 I=1,NCH
```

```
      DO 221 J=1,NCH
      IF(NWRT.GT.1) WRITE(6,907) I,J,PR(I,J),PR(J,I)
  911 FORMAT(F15.10)
      IF(ISKP.EQ.1.AND.IAS.EQ.2) GO TO 221
      IF(ISKP.EQ.2.AND.IAS.EQ.1) GO TO 221
      IF(ICAS.EQ.1.AND.KPUN.GT.0) WRITE(KPUN,909) I,J,PR(I,J)
      IF(ICAS.EQ.2.AND.KPUN.GT.0) WRITE(KPUN1,909) I,J,PR(I,J)
  221 CONTINUE
  909 FORMAT(2I5,F17.10)
  907 FORMAT(2I5,2E19.7)
      IF(NWRT.GT.0) WRITE(6,905)
C
C     CALCULATES EIGENPHASES AND SPIN WEIGHTED PARTIAL CROSS-SECTIOS :
C
      CALL CSEK2(PR,A1,NCH,0,KNK,BMQ,XIS,YYS,CCQ,DDQ)
      DO 222 I=1,NCH
      DO 222 J=I,NCH
      KIJ=I+(J*(J-1))/2
  222 ROS(KIJ)=(PR(I,J)+PR(J,I))/2.0
      CALL SIGEN(ROS,CSN,NCH,0,K2,KMMAX)
      SUM=0.0
      WRITE(6,1111)
 1111 FORMAT(11X,'EIGENPHASES',1X/)
      DO 23 I=1,NCH
      KII=I+(I*(I-1))/2
      STN=DATAN(ROS(KII))
      IF(NCH.EQ.1.AND.LT.EQ.0.AND.STN.LT.0)STN=STN+PI
      WRITE(6,906) I,STN
   23 SUM=SUM+STN
      WRITE(6,905)
      WRITE(6,2222)
 2222 FORMAT(11X,'EIGENPHASE SUM',1X/)
      WRITE(6,910) SUM
  910 FORMAT(5X,E19.7)
      WRITE(6,905)
      I=1
      WRITE(6,3333)
      WRITE(6,4444)
 3333 FORMAT(28X,'T MATRIX',1X/)
 4444 FORMAT(18X,'REAL PART',7X,'IMAGINARY PART',1X/)
      DO 1234 J=1,NCH
      WRITE(6,907)  I,J,XIS(I,J),YYS(I,J)
      IF(NPUN.GT.0) WRITE(7,1235) XIS(I,J),YYS(I,J),I,J,TK2
 1235 FORMAT(2F10.5,  25X,2I5,F10.5)
 1234 CONTINUE
      WRITE(6,905)
      ALQA=2.0*FLOAT(LT)+1.0
      ALQC=1.0
      IF(IAS.EQ.2)ALQC=3.0
      WRITE(6,5555)
 5555 FORMAT(16X,'CROSS SECTIONS ',1X//)
      DO 25 I=1,ICSMT
      ALQB=2.00* FLOAT(LAT(I))+1.00
      PPQ=ALQA*ALQC/(ALQB*TKS(I)*TKS(I))
      DO 24 J=1,NCH
      A1(I,J)=A1(I,J)*PPQ
   24 WRITE(6,904) I,J,A1(I,J)
   25 CONTINUE
      IF(ICAS.EQ.NCAS)GO TO 2002
      DO 26 I=1,NCH
```

```
      DO 26 J=1,NCH
      A1(I,J)=B0(I,J)
   26 A0(I,J)=B1(I,J)
 2001 WRITE(6,905)
 2002 WRITE(6,905)
 2003 CONTINUE
      RETURN
  904 FORMAT(2I5,E19.7)
  900 FORMAT(I5)
      END
```

```
      FUNCTION PHASE(L,ETA)
C*****************************************************************************
C     GENERATES THE COULOMB PHASE FOR ALL L AND ETA
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      C=0.577215664900
      N=1000
      SUM1=0.D0
      SUM2=0.D0
      DO 1 IS=1,N
      S=ETA/DFLOAT(IS)
    1 SUM1=SUM1+S-DATAN(S)
      SIGMA=-C*ETA+SUM1
      IF(L.EQ.0)GO TO 3
      DO 2 IS=1,L
    2 SUM2=SUM2+DATAN(ETA/DFLOAT(IS))
    3 PHASE=SIGMA+SUM2
      DN=N+1
      PHASE=PHASE+(ETA**3)/(6.D0*DN*DN)
      RETURN
      END
```

```
      SUBROUTINE SIGRN(A,R,N,NV,N2,NNMAX)
C*****************************************************************
C     WRITTEN BY DR J. CALLAWAY
C     N = ACTUAL DIMENSION
C     NMAX = MAXIMUM ORDINARY DIMENSION
C     N2 = NMAX*NMAX
C     NNMAX=(NMAX*(NMAX+1))/2
C     SET NV = 0 FOR NORMAL USE (EIGENVECTORS GENERATED)
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(NNMAX),R(N2)
    5 RANGR=1.D-10
      IF(NV-1) 10,25,10
   10 IQ=-N
      DO20J=1,N
      IQ=IQ+N
      DO20I=1,N
      IJ=IQ+I
      R(IJ)=0.0
      IF(I-J) 20,15,20
   15 R(IJ)=1.0
   20 CONTINUE
   25 ANORM=0.0
      DO35I=1,N
      DO35J=I,N
      IF(I-J) 30,35,30
   30 IA=I+(J*J-J)/2
      ANORM=ANORM+A(IA)*A(IA)
   35 CONTINUE
      IF(ANORM) 165,165,40
   40 ANORM=1.414*DSQRT(ANORM)
      ANRMX=ANORM*RANGE/FLOAT(N)
      IND=0
      THR=ANORM
   45 THR=THR/FLOAT(N)
   50 L=1
   55 M=L+1
   60 MQ=(M*M-M)/2
      LQ=(L*L-L)/2
      LM=L+MQ
   62 IF(DABS(A(LM))-THR) 130,65,65
   65 IND=1
      LL=L+LQ
      MM=M+MQ
      X=0.5*(A(LL)-A(MM))
   68 Y=-A(LM)/DSQRT(A(LM)*A(LM)+X*X)
      IF(X) 70,75,75
   70 Y=-Y
   75 SINX=Y/DSQRT(2.0*(1.0+(DSQRT(1.0-Y*Y))))
      SINX2=SINX*SINX
   78 COSX=DSQRT(1.0-SINX2)
      COSX2=COSX*COSX
      SINCS=SINX*COSX
      ILQ=N*(L-1)
      IMQ=N*(M-1)
      DO125I=1,N
      IQ=(I*I-I)/2
      IF(I-L) 80,115,80
   80 IF(I-M) 95,115,90
   85 IM=I+MQ
```

```
      GOTO95
90    IM=M+IQ
95    IF(I-L) 100, 105, 105
100   IL=I+LJ
      GOTO110
105   IL=L+IQ
110   X=A(IL)*COSX-A(IM)*SINX
      A(IM)=A(IL)*SINX+A(IM)*COSX
      A(IL)=X
115   IF(NV-1) 120,125,120
120   ILR=ILQ+I
      IMR=IMQ+I
      X=R(ILR)*COSX-R(IMR)*SINX
      R(IMR)=R(ILR)*SINX+R(IMR)*COSX
      R(ILR)=X
125   CONTINUE
      X=2.0*A(LM)*SINCS
      Y=A(LL)*COSX2+A(MM)*SINX2-X
      X=A(LL)*SINX2+A(MM)*COSX2+X
      A(LM)=(A(LL)-A(MM))*SINCS+A(LM)*(COSX2-SINX2)
      A(LL)=Y
      A(MM)=X
130   IF(M-N) 135, 140, 135
135   M=M+1
      GOTO60
140   IF(L-(N-1)) 145,150,145
145   L=L+1
      GOTO55
150   IF(IND-1) 160,155,160
155   IND=0
      GOTO50
160   IF(THR-ANORM) 165,165,45
165   IQ=-N
      DO185I=1,N
      IQ=IQ+N
      LL=I+(I*I-I)/2
      JQ=N*(I-2)
      DO185J=I,N
      JQ=JQ+N
      MM=J+(J*J-J)/2
      IF(A(LL)-A(MM)) 170,185,185
170   X=A(LL)
      A(LL)=A(MM)
      A(MM)=X
      IF(NV-1) 175,185,175
175   DO180K=1,N
      ILR=IQ+K
      IMR=JQ+K
      X=R(ILR)
      R(ILR)=R(IMR)
180   R(IMR)=X
185   CONTINUE
      RETURN
      END
```

```
      DOUBLE PRECISION FUNCTION S6J(JD1,JD2,JD3,LD1,LD2,LD3)
C*****************************************************************************
C     VERSION II  FORTRAN IV
C     WRITTEN BY DR. J.CALLAWAY.REVISED FEB. 1976
C     GENERATES 6J-SYMBOLS
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*4 SNGL
      DIMENSION MA(4),MB(3),MED (12)
      DIMENSION FL(400)
      DFLOAT(I)=I
      J1=JD1
      J2=JD2
      J3=JD3
      L1=LD1
      L2=LD2
      L3=LD3
C
C     DETERMINE WHETHER TO CALCULATE FL(N) S
C
      IF(NCALL+1867) 5,15,5
    5 NCALL=-1867
C
C     CALCULATE FL(N) S
C
      FL(1)=0.0D0
      FL(2)=0.0D0
      DO 50 N= 3,322
      FN=DFLOAT(N-1)
   50 FL(N)=FL(N-1)+DLOG(FN)
   15 MED(1)=(-J1+J2+J3)/2
      MED(2)=(+J1-J2+J3)/2
      MED(3)=(+J1+J2-J3)/2
      MED(4)=(-J1+L2+L3)/2
      MED(5)=(+J1-L2+L3)/2
      MED(6)=(+J1+L2-L3)/2
      MED(7)=(-L1+J2+L3)/2
      MED(8)=(+L1-J2+L3)/2
      MED(9)=(+L1+J2-L3)/2
      MED(10)=(-L1+L2+J3)/2
      MED(11)=(+L1-L2+J3)/2
      MED(12)=(+L1+L2-J3)/2
      MA(1)=MED(1)+MED(2)+MED(3)
      MA(2)=MED(4)+MED(5)+MED(6)
      MA(3)=MED(7)+MED(8)+MED(9)
      MA(4)=MED(10)+MED(11)+MED(12)
      MB(1)=MA(1)+MED(12)
      MB(2)=MA(1)+MED(4)
      MB(3)=MA(1)+MED(8)
C
C     DETERMINE MAXIMUM OF (J1+J2+J3),(J1+L2+L3),(L1+J2+L3),(L1+L2+J3)
C
      MAX=MA(1)
      DO 30 N=2,4
      IF (MAX-MA(N)) 20,30,30
   20 MAX=MA(N)
   30 CONTINUE
C
C     DETERMINE MINIMUM OF (J1+J2+L1+L2), (J2+J3+L2+L3),(J3+J1+L3+L1)
C
```

```
      MIN=MB(1)
      DO 51 N=2,3
      IF (MIN-MB(N)) 51,51,40
   40 MIN=MB(N)
   51 CONTINUE
      KMAX=MIN-MAX
      MINP1=MIN+1
      MIN1  =MINP1-MA(1)
      MIN2=MINP1-MA(2)
      MIN3=MINP1-MA(3)
      MIN4=MINP1-MA(4)
      MIN5=MINP1+1
      MIN6=MB(1)-MIN
      MIN7=MB(2)-MIN
      MIN8=MB(3)-MIN
C
C     SUM SERIES IN DOUBLE PRECISION
C
      UK=1.D-15
      S=1.0D-15
      IF (KMAX) 65,65,55
   55 DO 60 K=1,KMAX
      UK=-UK*DFLOAT(MIN1-K)*DFLOAT(MIN2-K)*DFLOAT(MIN3-K)*DFLOAT(MIN4-K)
     1/(DFLOAT(MIN5-K)*DFLOAT(MIN6+K)*DFLOAT(MIN7+K)*DFLOAT(MIN8+K))
C
C     CUT OFF SERIES AT 1.0E-25
C
      IF(DABS(UK)-1.D-25) 65,65,60
   60 S=S+UK
   65 S=S*1.0D+15
C
C     CALCULATE DELTA FUNCTIONS
C
      DELOG=0.0D0
      DO 70 N=1,12
      NUM=NED(N)
   70 DELOG=DELOG+FL(NUM+1)
      NUM1=MA(1)+2
      NUM2=MA(2)+2
      NUM3=MA(3)+2
      NUM4=MA(4)+2
      DELOG=DELOG-FL(NUM1)-FL(NUM2)-FL(NUM3)-FL(NUM4)
      DELOG=0.5D0*DELOG
      ULOG=FL(MIN5)-FL(MIN1  )-FL(MIN2)-FL(MIN3)-FL(MIN4)-FL(MIN6+1)- FL
     1(MIN7+1)-FL(MIN8+1)
      PLOG=DELOG+ULOG
      IF(SNGL(PLOG)+64.0) 72,75,75
   72 Q=PLOG+64.D0
      Q=DEXP(Q)
      S6J=Q*S
      IF(DABS(S6J)-1.D0)  73,73,74
   73 S6J=0.D0
      GO TO 90
   74 S6J=S6J*DEXP(-64.D0)
      GO TO 78
   75 P=DEXP(PLOG)
      S6J =P*S
   78 MIN2=MIN/2
      IF (MIN-2*MIN2) 80,90,80
   80 S6J=-S6J
```

```
90 CONTINUE
   RETURN
   END
```

```
      FUNCTION XCOR(II,IJ,LQ)
C*****************************************************************
C     COMPUTES INTEGRALS OF THE TYPE : INT(R-INFINITY) OF
C              C(LP,P)*C(LQ,Q)/X**(LQ+1)    ,LQ=1,2,....
C     C(LP,P)  IS EITHER A SINE OR COSINE OF :
C              P*X - EP*LOG(2*P*X) - LP*PI/2 +SIGMA(LP,P) ,
C     IN WHICH EP IS THE COULOMB PARAMETER & SIGMA IS THE COULOMB PHASE
C     Z IS THE NUCLEAR CHARGE
C     REMARK :  C(LQ,Q)  IS DEFINED LIKEWISE
C*****************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      COMPLEX*16 SIGMA,DELTA,SPQ,DPQ,U,SUMG,SUMD,SUM,DIFF,GK
      COMMON/CRR/P,Q,Z,R,LP,LQ
      EP=-(Z-1.D0)/P
      EQ=EP*P/Q
      U=DCMPLX(0.D0,1.D0)
      PI=3.141592653589D0/2.D0
      DLGP=EP*DLOG(2.D0*P)
      SIGLP=PHASE(LP,EP)
      IF(LP.EQ.LQ.AND.P.EQ.Q)GO TO 1
      DLP=DATAN(EP/DFLOAT(LP+1))
      IF(LQ.EQ.(LP+1).AND.P.EQ.Q)GO TO 2
      SIGLQ=PHASE(LQ,EQ)
      DLGQ=EQ*DLOG(2.D0*Q)
      DLQ=DATAN(EQ/DFLOAT(LQ+1))
      IF(LP.EQ.(LQ+1).AND.P.EQ.Q)GO TO 3
      SPQ=DCMPLX(0.D0,SIGLP+SIGLQ-PI*DFLOAT(LP+LQ)-DLGP-DLGQ)
      DPQ=DCMPLX(0.D0,SIGLP-SIGLQ-PI*DFLOAT(LP-LQ)-DLGP+DLGQ)
      SIGMA=CDEXP(SPQ)
      DELTA=CDEXP(DPQ)
      GO TO 4
    1 DELTA=DCMPLX(1.D0,0.D0)
      SPQ=DCMPLX(0.D0,2.D0*(SIGLP-DLGP))
      SPQ=CDEXP(SPQ)
      SIGMA=SPQ*DCMPLX((-1.D0)**LP,0.D0)
      GO TO 4
    2 DPQ=DCMPLX(0.D0,-DLP)
      DELTA=U*CDEXP(DPQ)
      SPQ=DCMPLX(0.D0,2.D0*(SIGLP-DLGP)+DLP)
      SPQ=CDEXP(SPQ)
      SIGMA=U*SPQ*DCMPLX((-1.D0)**(LP+1),0.D0)
      GO TO 4
    3 DPQ=DCMPLX(0.D0,DLQ)
      DELTA=-U*CDEXP(DPQ)
      SPQ=DCMPLX(0.D0,2.D0*(SIGLQ-DLGQ)+DLQ)
      SPQ=CDEXP(SPQ)
      SIGMA=U*SPQ*DCMPLX((-1.D0)**(LQ+1),0.D0)
    4 SUMG=SIGMA*GK(LR,R,EP+EQ,P+Q)
      SUMD=DELTA*GK(LR,R,EP-EQ,P-Q)
      SUM=0.5D0*(SUMG+SUMD)
      DIFF=0.5D0*(SUMG-SUMD)
      IF(II.EQ.1) GO TO 6
      IF(IJ.EQ.1)GO TO 5
      XCOR=-DREAL(DIFF)
      RETURN
    5 XCOR=DIMAG(SUM)
      RETURN
    6 IF(IJ.EQ.1)GO TO 7
      XCOR=DIMAG(DIFF)
      RETURN
```

```
7 XCOR=DREAL(SUM)
  RETURN
  END
```

```
      FUNCTION XIP(I1,N1,J1,Z1,B1,IM)
C*****************************************************************************
C     EVALUATES NUMERICALLY INTEGRALS OF THE TYPE : INT(0-R(IM)) OF
C              (X**N1)*EXP(-Z1*X)*((1-EXP(-B1*X))**J1)*(FQ OR GQ)
C     FQ & GQ ARE RESPECTIVELY THE REGULAR & IRREGULAR COULOMB FUNCTIONS
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION R(1200),F(1200)
      COMMON/RODE/DELR,R,NN
      COMMON/FIF/FQ(1200),GQ(1200)
      DO 2 I=1,IM
      B1R=-B1*R(I)
      Z1R=-Z1*R(I)
      V=R(I)**N1*DEXP(Z1R)
      IF(J1.NE.0)  V=V*(1.D0-DEXP(B1R))**J1
      IF(I1.EQ.0)  F(I)=V*FQ(I)
      IF(I1.EQ.1)  F(I)=V*GQ(I)
    2 CONTINUE
      CALL BINT(IM,F,DELR,Y)
      XIP=Y
      RETURN
      END
```

```
      FUNCTION XK12(N,A,M,B,L,R)
C*************************************************************************
C     CALCULATES INTEGRALS OF THE TYPE :INT(0-INF.) OF :
C     (X**N)*EXP(-A*X)*(X**M)*EXP(-B*X)*(R<**L/R>**(L+1))
C*************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      LIM=M+N+L+2
      AB=A+B
      Y=DFACTR(LIM)/(AB**(LIM+1)*R**(L+1))
      SUM=0.D0
      DO 1 NU=1,LIM
      IN=NU-1
    1 SUM=SUM+AITCH(N,M,L,IN,A,B)*R**IN
      XK12=Y*(1.D0-SUM*DEXP(-AB*R))
      RETURN
      END
```

```
      FUNCTION XL(IX,Y)
C*****************************************************************************
C     COMPUTES INTEGRALS OF THE FORM:INT(0-INF.) OF (R**X)*EXP(-Y*R)*
C    L(R),WHERE L(R) IS THE L=0 REGULAR COULOMB FUNCTION
C     L(R) BEHAVES AS R**L AS R GOES TO 0.(F(R)=TK*R*L(R))
C    TK IS THE WAVE VECTOR IN RYDBERGS
C     A IS THE COULOMB PARAMETER
C    XN IS THE NORMALIZATION OF THE FREE COULOMB FUNCTION
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION XP(50)
      COMMON/ANL/TK,AX
      PI=3.14159265358979300
      PI=PI*2.D0*AX
      XN=PI/(DEXP(PI)-1.D0)
      XN=DSQRT(XN)
      A=AX
      N=IX+1
      E=TK*TK
      AK=A*TK
      TY=TK/Y
      YE=E+Y**2
      PHI=2.D0*DATAN(TY)
      AP=A*PHI
      DAP=DEXP(AP)
      XP(1)=(DAP-1.D0)/(2.D0*TK*A)
      IF(IX.NE.0) GO TO 1
      XL=XP(1)*XN
      RETURN
    1 XP(2)=DAP/YE
      IF(IX.NE.1) GO TO 2
      XL=XP(2)*XN
      RETURN
    2 DO 10 I=3,N
      DI=DFLOAT(I)
      XP(I)=(2.D0*(AK+Y*(DI-2.D0))*XP(I-1)-
     1(DI-2.D0)*(DI-3.D0)*XP(I-2))/YE
   10 CONTINUE
      XL=XN*XP(IX+1)
      RETURN
      END
```

```
      FUNCTION XLJ(L,N,A)
C*************************************************************************
C     COMPUTES INTEGRALS OF THE TYPE : INT(0-INFINITY) OF
C          (R**N)*EXP(-A*R)*F(L,AX,TK*R),
C     F BEING THE REGULAR COULOMB FUNCTION AND AX  THE COULOMB PARAMETR.
C*************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/ANL/TK,AX
      IF(L.GT.0)GO TO 1
      XLJ=TK*XL(N+1,A)
      RETURN
    1 M=N+L+2
      XLJ=XLM(L,N,M,A)
      RETURN
      END
```

```
      FUNCTION XLM(L,N,M,A)
C*****************************************************************************
C     COMPUTES INTEGRALS OF THE TYPE : INT(0-INFINITY) OF
C              (R**N)*EXP(-A*R)*F(L,AX,TK*R)   ,  FOR L GE. 1
C      F IS THE REGULAR COULOMB FUNCTION AND AX IS THE COULOMB PARAMETER
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X(20,100),AL(20),BL(20),CL(20)
      COMMON/ANL/TK,AX
      DO 1 I=1,L
      DI=I
      AL(I)=1.D0/(TK*DSQRT(DI*DI+AX*AX))
    1 BL(I)=AX*TK-A*DI
      E=A*A+TK*TK
      AK=-2.D0*AX*TK
      XLL=XL(0,A)
      DO 2 I=1,L
      CALL NOBM(I-1,AX,XN)
    2 CL(I)=XN
      X(1,1)=0.5D0*TK*AL(1)*((E+AK*BL(1))*XLL+E*BL(1)*XL(1,A)+AK*CL(1))
      IF(L.EQ.1.AND.N.EQ.-2)GO TO 7
      X(1,2)=TK*AL(1)*(BL(1)*XLL+CL(1))
      IF(L.EQ.1.AND.N.EQ.-1)GO TO 7
      IF(L.LT.2.AND.N.GE.0)GO TO 4
      DO 3 I=2,L
      DI=I
      X(I,1)=(AL(I)/(2.D0*DI))*((DI*E-2.D0*BL(I)*BL(I-1))*X(I-1,1)+
     1       BL(I)*E*X(I-1,2)-2.D0*DI*CL(I)*BL(I-1)*TK**I)
      IF(I.EQ.L.AND.N.EQ.(-L-1))  GO TO 7
      X(I,2)=AL(I)*(BL(I)*X(I-1,1)+DI*CL(I)*TK**I)
      IF(I.EQ.L.AND.N.EQ.-L)GO TO 7
    3 CONTINUE
    4 DO 5 K=3,M
      LAM=K-L-2
    5 X(L,K)=(2.D0*(AX*TK+A*DFLOAT(LAM))*X(L,K-1)+DFLOAT(L*(L+1)
     1       -LAM*(LAM-1))*X(L,K-2))/E
    7 XLM=X(L,M)
      RETURN
      END
```

```
**********INPUT DATA FOR MAIN1**********

  40   40                      NCHMX        NCAT
   T    F    T    F    F      IRED JPUN JWRT ITAPE IDISK
   0                           L
   8                           NZCH
 0.00010                       RMN
30.00010                       RMAX
 701                           NPTS
   2                           NATL
   3                           NBSAZ(1)
   3                           NBSAZ(2)

NT(I,J)  NNN          ENEG(I,J)

   3     0     -0.10000000000000D+01
   3     0     -0.25000000000000D+00
   3     0      0.31115107913668D+00
   3     1     -0.25000000000000D+00
   3     1     -0.21454695859559D-01
   3     1      0.11255626540272D+01

NPNR(I,J)    Z(I,J)

   0    1.00000000000000
   0    0.50000000000000
   1    0.50000000000000
   1    1.00000000000000
   1    0.50000000000000
   1    0.80000000000000

NPNB(I,J)     Z(I,J)          CEIG(I,J,M)

   0    1.00000000000000   2.00000000000000
   0    0.50000000000000  -0.00000000000000
   1    0.50000000000000  -0.00000000000000
   0    1.00000000000000   0.00000000000000
   0    0.50000000000000  -0.70710677365363
   1    0.50000000000000   0.35355339125138
   0    1.00000000000000   7.67692984197207
   0    0.50000000000000  -4.85805716562293
   1    0.50000000000000   0.80967619427049
   1    1.00000000000000   0.00000000000000
   1    0.50000000000000   0.20412414523193
   1    0.80000000000000   0.00000000000000
   1    1.00000000000000  -3.09507740731253
   1    0.50000000000000  -0.56870094249616
   1    0.80000000000000   3.61998155031467
   1    1.00000000000000  -8.03334879420980
   1    0.50000000000000  -0.46593429367283
   1    0.80000000000000   5.65785127557263

  0                          ILLI
 15                          NSTO

 ZPTA(I)

15.60000
12.00000
 9.23077
```

```
   7.10059
   5.46199
   4.20153
   3.23195
   2.48611
   1.91240
   1.47107
   1.13160
   0.87046
   0.66958
   0.51506
   0.39620

 -14.0800                    E,TOTAL ENERGY
   2.4                       GAMMA

******************INPUT DATA FOR MAIN3************************************

    2    1    1              IWRT      NE       IPIPH
    3   10    0              NPST      KPUN      ISKP

******************INPUT DATA FOR MAIN4************************************

    3    0    1    1    1    NWRT  NPUN  NE  ICWST  IOMN
    3    2    0              NPST  KPUN  ISKP
```

```
MAX. # OF CHANNELS  MAX. # OF OPEN CHANNELS  MAX. DIMENSION OF BOUND-BOUND MATRIX  MAX. DIMENSION OF PSEUDOBASIS

      40                  40                  866                                  10
CHANNEL INDICES OF THE LAST FF. ELEMENT(CALCULATED &  STORED ON DISC;UNIT 9)

   2    2    1    1
NUCLEAR CHARGE=   8.00000

R MAX.=  30.00010

MESH SIZE=   0.04286

NUMBER OF MESHES=  701

ACTUAL MAX. # OF CHANNELS=    6

ACTUAL # OF OPEN CHANNELS=    3

ACTUAL DIMENSION OF THE BB. MATRIX=      90

CORRECTED DIMENSION OF BB. MATRIX=   90

LNX=NDIM*(NDIM+1)/2=    4095

    PSEUDOSTATE ANG. MOM.  # OF PSEUDOSTATES FOR A SPECIFIC L     CHANNEL ANG MOM          CHANNEL ENERGY(IN RY)

  1              0                        1                      0                      49.92000
  2              0                        2                      0                       1.92000
  3              0                        3                      0                       0.0
  4              1                        1                      1                       1.92000
  5              1                        2                      1                       0.0
  6              1                        3                      1                       0.0

SHORT RANGE BASIS EXPONENTS(ZETA)

   1    0.156000000000000D+02
   2    0.120000000000000D+02
   3    0.923077000000000D+01
   4    0.710059000000000D+01
   5    0.546199000000000D+01
   6    0.420153000000000D+01
   7    0.323195000000000D+01
   8    0.248611000000000D+01
   9    0.191248000000000D+01
  10    0.147107000000000D+01
  11    0.113160000000000D+01
  12    0.870460000000000D+00
  13    0.669580000000000D+00
  14    0.515060000000000D+00
  15    0.396200000000000D+00

TOTAL ENERGY  GAMMA  INCIDENT ENERGY

-14.080000   2.400000  49.920000
```

CALCULATED AND STORED FF. MATRIX ELEMENTS :

1	1	1	1	1	-0.7863027867848120+00	-0.1283404847763180-01	0.7052574648286D+01	0.3178771786752D+00
1	1	1	1	2	0.2330858270023700+00	0.1081861768933800+00	0.1081861768933800+00	-0.2515755776777D+00
1	1	2	1	1	0.7073642567719600-01	-0.1042745865838900-01	0.6962248238361300-02	0.6763722150086D-02
1	1	2	1	2	0.4380964757085100-01	0.7758071624520200-01	0.4301927107690400-01	-0.1617512927883D+00
1	1	4	1	1	0.5823456856380900-01	-0.8977618215017500-02	0.1381801889402D-01	0.1396747476896D-02
1	1	4	1	2	0.4106094892560900-01	-0.5726806740213900-02	0.7659504408807600-03	0.2530223418824D-02
2	1	2	1	1	-0.3978193719108900+00	-0.1091827206810600-02	0.1384589218848300+01	0.3560899573122600-01
2	1	2	1	2	0.2678919739919800-01	0.1193099797850700+00	0.1193099797850700+00	-0.3112319112716900+00
2	1	4	1	1	-0.2599568673920000+00	-0.1213016687754600+00	0.9859967851469600-01	-0.2006777488118800+00
2	1	4	1	2	-0.2885511304706900-01	-0.2132271227137700-01	0.2748690525656700-01	-0.1985961578054500-01
4	1	4	1	1	-0.1104638309175000+00	-0.2818360692182400-02	0.1381227628536290+01	0.1506650343054900+00
4	1	4	1	2	0.1240619604910200+00	0.3016685622993800-01	0.3016685622993800-01	-0.6331425189308900-01

COUNTERS FOR BB.,BF.,AND FF. ELEMENTS :

8185 560 36

SINGLET EIGENVALUES COUNT 30

TRIPLET EIGENVALUES COUNT 29

TOTAL ANGULAR MOMENTUM INCIDENT ENERGY # OF OPEN CHANNELS TOTAL # OF CHANNELS

0 49.9200030 2 6

ANGULAR MOMENTA OF PSEUDOSTATES :

0 0 0 1 1 1

CHANNEL ENERGIES :

1 7.0454006933A220
2 1.3854006A4055110
3 -5.0304008996135240
4 1.3854006A4055110
5 -3.5A46738233B5111
6 -9.279871218B8990

SINGLET

DETM : REAL INVERSE REAL

0.5820358180D-01 -0.8237090609D+00

R MATRIX REAL INVERSE REAL

1 1 0.773332338D-01 0.7729840328D-01
1 2 -0.3196662478D-01 -0.3895911178D-01
1 3 -0.3665193688D-01 -0.2641828798D-01
2 1 -0.3196662478D-01 -0.3895911178D-01
2 2 0.2476911788D+00 0.2273685298D+00
2 3 0.2172597738D+00 0.2377882988D+00
3 1 -0.3665193688D-01 -0.2641828798D-01
3 2 0.2172597738D+00 0.2377882988D+00
3 3 0.1315406A48D-01 0.1554985618D-01

T MATRIX ELEMENTS REAL

		REAL PART	IMAGINARY PART	INVERSE REAL PART	INVERSE IMAGINARY PART
1	1	0.7A6038152D-01	0.826653A08D-02	0.7536877348-01	0.8256792108D-02
1	2	-0.3202568968D-01	-0.1782598218-01	-0.3288548/448-01	-0.1788655858D-01
1	3	-0.3197786358-01	-0.1879883898-01	-0.3190675568D-01	-0.1887852788-01

EIGENPHASES : REAL INVERSE REAL

1 0.2715710880D+00 0.2722979408D+00
2 0.6879544198-01 0.6817669768-01
3 -0.1394877868D+00 -0.1383140818D+00

EIGENPHASE SUMS

0.3808799569D+00 0.3827579518+00

CROSS SECTIONS REAL INVERSE REAL

1 1 0.1150A84198D-02 0.1157612698-01

1	2	0.2n91858110-04	0.26n70n4510-04
1	3	0.2201660060-04	0.227600e050-04
2	1	0.4996740n90-03	0.6984128720-03
2	2	0.2n2552n050-01	0.2416311110-01
2	3	0.2n970164970-01	0.2505702760-01
3	1	0.1n778n3650-03	0.1972585810-03
3	2	0.8123180990D-02	0.8135234250-02
3	3	0.4651899060-03	0.4695269080-03

TRIPLET

BETA : SOMM INVERSE SOMM

-0.2328755930-01 -0.1065272090+01

K MATRIX SOMM INVERSE SOMM

1	1	0.1532n303100+00	0.1530213380+00
1	2	-0.2n19731680D-02	-0.2392132610-02
1	3	-0.7195250100-02	-0.7982720700-02
2	1	-0.2519731680D-02	-0.2392132610-02
2	2	0.3n06127650+00	0.3023117840+00
2	3	0.1n03285790+00	0.1915540470+00
3	1	-0.7195250100-02	-0.7982720700-02
3	2	0.1n03285790+00	0.1915540470+00
3	3	0.2836n69370+00	0.1971978020+00

T MATRIX ELEMENTS SOMM INVERSE SOMM

		REAL PART	IMAGINARY PART	REAL PART	IMAGINARY PART
1	1	0.1n969720330+00	0.2298747860-01	0.1n998530n90+00	0.2293187660-01
1	2	-0.1296151690-02	-0.1985044230-02	-0.1106795130-02	-0.2051038370-02
1	3	-0.6128153570-02	-0.2572829240-02	-0.6862785210-02	-0.2758630200-02

IGENPHASES : SOMM INVERSE SOMM

1	0.n030704870+00	0.n032211n80+00
2	0.1521739580+00	0.1520152370+00
3	0.6953n30030-01	0.6945225040-01

IGENPHASE SUMS

0.6447787450+00 0.6597589620+00

CROSS SECTIONS SOMM INVERSE SOMM

1	1	0.1378666860-02	0.1376501550-02
1	2	0.3177650890-06	0.3264221960-06
1	3	0.2654023110-05	0.3207732050-05
2	1	0.8781902710-05	0.8806977080-05
2	2	0.1486824130+00	0.1500051610+00
2	3	0.4597240580-01	0.4659010720-01
3	1	0.2100450010-06	0.2849167740-06
3	2	0.1532n13530-01	0.1553001570-01
3	3	0.1481539890-01	0.1686019670-01

```
# OF CHANNELS  TOTAL # OF CHANNELS  TOTAL ANGULAR MOMENTUM

      3                6                  0

CHANNEL ENERGIES


       7.06540869306220
       1.38564064605510
      -5.81040899635288
       1.38564064605510
      -3.56467382306511
      -9.27987121988990

ANGULAR MOMENTA OF PSEUDOSTATES :

  0   0   0   1   1   1

INCIDENT ENERGY

     0.49920000D+02

  SINGLET


OMN RESULTS


DET(M) :

    -0.62371650-01

                          K MATRIX

   1    1      0.7730887D-01      0.7730887D-01
   1    2     -0.3897261D-01     -0.3897261D-01
   1    3     -0.3660239D-01     -0.3660239D-01
   2    2      0.2276710D+00      0.2276710D+00
   2    3      0.2376010D+00      0.2376010D+00
   3    3      0.1345398D-01      0.1345398D-01

         EIGENPHASES

   1      0.1718925D+00
   2      0.6882059D-01
   3     -0.1395839D+00

         EIGENPHASE SUM

         0.3011292D+00

                          T MATRIX

                REAL PART          IMAGINARY PART

   1    1      0.7561941D-01      0.8265524D-02
   1    2     -0.3202519D-01     -0.1782247D-01
```

1	3	-0.3191983D-01	-0.1080652D-01

CROSS SECTIONS

1	1	0.1159178D-03
1	2	0.2690812D-04
1	3	0.2274952D-04

IOHH RESULTS

DET(M) :

-0.1373946D-06

K MATRIX

1	1	0.7730178D-01	0.7730178D-01
1	2	-0.3890245D-01	-0.3890245D-01
1	3	-0.3667066D-01	-0.3667066D-01
2	2	0.2288657D+00	0.2288657D+00
2	3	0.2378899D+00	0.2378899D+00
3	3	0.1489701D-01	0.1489701D-01

EIGENPHASES

1	0.3731786D+00
2	0.6081121D-01
3	-0.1385075D+00

EIGENPHASE SUM

0.3035023D+00

T MATRIX

		REAL PART	IMAGINARY PART
1	1	0.7557176D-01	0.8255525D-02
1	2	-0.3191772D-01	-0.1784790D-01
1	3	-0.3196060D-01	-0.1084029D-01

CROSS SECTIONS

1	1	0.1157701D-03
1	2	0.2678861D-04
1	3	0.2281634D-04

TRIPLET

OHH RESULTS

DET(M) :

0.2529201D+00

K MATRIX

1	1	0.1530177D+00	0.1530177D+00
1	2	-0.2278355D-02	-0.2278355D-02
1	3	-0.7254149D-02	-0.7254149D-02
2	2	0.3406551D+00	0.3406551D+00
2	3	0.1906446D+00	0.1906446D+00
3	3	0.2041004D+00	0.2041004D+00

EIGENPHASES

1	0.4434428D+00
2	0.1519796D+00
3	0.6950718D-01

EIGENPHASE SUM

0.6649296D+00

T MATRIX

		REAL PART	IMAGINARY PART
1	1	0.1494874D+00	0.2292172D-01
1	2	-0.1092543D-02	-0.1895564D-02
1	3	-0.6204205D-02	-0.2558972D-02

CROSS SECTIONS

1	1	0.1374513D-02
1	2	0.2976690D-06
1	3	0.2706761D-05

IOHN RESULTS

DET(M) :

0.7438319D-07

K MATRIX

1	1	0.1530554D+00	0.1530554D+00
1	2	-0.2293965D-02	-0.2293965D-02
1	3	-0.7418268D-02	-0.7418268D-02
2	2	0.3408175D+00	0.3408175D+00
2	3	0.1905747D+00	0.1905747D+00
3	3	0.2033897D+00	0.2033897D+00

EIGENPHASES

1	0.4432892D+00
2	0.1520257D+00
3	0.6913938D-01

EIGENPHASE SUM

0.6644543D+00

T MATRIX

		REAL PART	IMAGINARY PART
1	1	0.1495213D+00	0.2293466D-01
1	2	-0.1088444D-02	-0.1924280D-02
1	3	-0.6350906D-02	-0.2608328D-02

CROSS SECTIONS

1	1	0.1375158D-02
1	2	0.2937237D-06
1	3	0.2832776D-05

VITA

Najib AbuSalbi was born on November 11, 1953 in Beirut, Lebanon. He graduated from Kfarshima National Secondary School, Kfarshima, Lebanon, in 1971. He received the degree of License in Physics from the Lebanese University, Beirut, Lebanon, in 1974. In December 1976, he transferred from the American University of Beirut, Lebanon, to Louisiana State University, Baton Rouge, Louisiana, for post-graduate studies and received the degree of Master of Science in January 1978. He is now a candidate for the degree of Doctor of Philosophy in the Department of Physics and Astronomy at Louisiana State University.

He is a member of the American Physical Society and of the American Association of Physics Teachers.

EXAMINATION AND THESIS REPORT

Candidate: Najib Nimer AbuSalbi

Major Field: Atomic Physics

Title of Thesis: "Scattering of Electrons by Hydrogenic Ions"

Approved:

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

Date of Examination:

July 13, 1981